QUANTUM MECHANICS AND MANY-BODY PROBLEMS

EFFECTIVE OPERATORS IN ATOMIC ENERGY LEVEL Z-EXPANSION CALCULATIONS

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by

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To my wife

ABSTRACT

Rajnak and Wybourne's effective operators are generalized to degenerate ground configurations ℓ^N and $\ell'^{4\ell'}\ell^{N+2}$ as well as by removing the assumption of a Hartree-Fock basis. Explicit calculation of discrete radial integrals and energy denominators permits calculation of the discrete part of E_2 in Layzer's Z-expansion. Specific application is made to the carbon isoelectronic sequence. Ground state energies obtained are not as low as Hartree-Fock values, but term structure prediction is better. Continuum contributions are estimated to be fifteen percent of E_2.

First and second-order fine structure calculations are too large. Reasons why third-order is expected to be important are given.

The possibility of Z-expansions with non-hydrogenic basis is considered.

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CONTENTS

INTRODUCTION

Rajnak and Wybourne[1-3] have shown that it is possible to represent the effects of perturbation theory by a series of effective operators acting on the zero-order states. They calculated the effective operators, to second-order, for a single open orbital of N equivalent electrons ℓ^N on the assumption that the zero-order functions are Hartree-Fock. The angular part of the effective operators were calculated exactly for species of excited configurations which contribute to the term structure. Associated radial integrals and energy denominators were considered to be incorporated into a small set of parameters to be determined from experimental data.

We shall generalize this work to degenerate ground configurations ℓ^N and $\ell'^4\ell'\ell^{N+2}$ removing the assumption of a Hartree-Fock basis. By explicit calculation of radial integrals and energy denominators we will apply this theory to evaluation of the third term E_2 in Layzer's[4,5] Z-expansion.

The Z-expansion being a direct consequence of taking hydrogenic basis functions permits an analytic treatment of the discrete states. Advantages and disadvantages of such functions are studied and the connection with the Hartree-Fock scheme is explained.

Specific application is made to the carbon isoelectronic sequence for the Coulomb repulsion and fine structure. The importance of continuum states and the possibility of other zero-order functions is considered.

CHAPTER 1

PERTURBATION THEORY AND THE Z-EXPANSION

1.1 INTRODUCTION

In this chapter we shall introduce the notation used in later sections. A brief review of Rayleigh-Schrödinger and operator perturbation theory is given and their relationship to the effective operator techniques of Rajnak and Wybourne is discussed. Finally, the basic ideas of the Z-expansion to the many-electron atom is given.

1.2 THE MANY-ELECTRON ATOM

According to Rutherford's nuclear model we regard the atom as made up of a central massive positively charged nucleus surrounded by electrons.

The nuclear mass being at least 1800 times that of the electron is approximated as a fixed force centre. The non-relativistic Hamiltonian for N electrons of charge e, mass m moving about a fixed point nucleus of charge Ze is[6]

$$H_{NR} = \sum_{i=1}^{N} \left(\frac{\underset{\sim}{p}_i^2}{2m} - \frac{Ze^2}{r_i}\right) + \sum_{i<j} \frac{e^2}{r_{ij}}$$

where r_i is the distance between electron i and the nucleus, $\underset{\sim}{p}_i$ is the linear momentum operator for electron i, and r_{ij} is the separation of electrons i and j. Electrons interact in pairs, and as we wish to include each pair just once, the last sum is over all distinct pairs of electrons.

We shall use Hartree's atomic units[6,7] in which m, $\hbar$ and e are taken as unity. In these units

$$H_{NR} = \sum_{i=1}^{N} \left(\frac{\underset{\sim}{p}_i^2}{2} - \frac{Z}{r_i}\right) + \sum_{i<j} \frac{1}{r_{ij}} \qquad (1.1)$$

The single-particle relativistic corrections to H_{NR} are obtained by carrying out a Foldy-Wouthuysen-Tani[8] transformation on the Dirac Hamiltonian for an electron moving in an external electromagnetic field. The largest single-particle correction is the spin-orbit interaction, first suggested by Thomas[9] and Frenkel[10] on considering the electron as a spinning top. In tensorial notation the spin-orbit operator is (in a.u.)

$$\frac{1}{2c^2 r}\frac{\partial U}{\partial r}\,(\underset{\sim}{s}^{(1)}\cdot\underset{\sim}{\ell}^{(1)}) \qquad (1.2)$$

where U is the symmetric electrostatic field the electron moves in. Two-particle relativistic corrections are introduced via the spin-spin, spin-other-orbit and magnetic hyperfine interactions.

The free atom is observed to have inversion symmetry, consequently its Hamiltonian must exhibit this invariance.

Hamiltonian H_{NR} commutes with the total orbital angular momentum operator $\underset{\sim}{L} = \sum_i \underset{\sim}{\ell}_i$, the total spin operator $\underset{\sim}{S} = \sum_i \underset{\sim}{s}_i$, and the space inversion operator. Eigenfunctions of H_{NR} may therefore be labelled by the good quantum numbers p(parity)SL and written as $|\gamma pSLM_S M_L\rangle$, γ being any other quantum numbers required to uniquely label the wavefunctions. We call $|\gamma pSLM_S M_L\rangle$ a state and the (2S+1)(2L+1) states labelled $|\gamma pSL\rangle$ are called terms.

On including the spin-orbit operator SL are no longer good quantum numbers, but the total angular momentum $\underset{\sim}{J} = \underset{\sim}{S} + \underset{\sim}{L}$ is. Now the terms split into levels labelled $|\gamma pSLJ\rangle$. This description assumes that the spin-orbit interaction is much smaller than the Coulomb. If this is not so SL are not even

approximately conserved and the wavefunction is a linear sum of terms.

1.3 CENTRAL FIELD APPROXIMATION

Eigenvalue problem

$$H_{NR}\Psi = E_{NR}\Psi \tag{1.3}$$

is unsolvable because of the $\Sigma \frac{1}{r_{ij}}$ term, forcing us to consider approximate methods.

The electron-electron term is not small since for an N-electron atom there are $\frac{1}{2}N(N-1)$ pairs of interacting electrons, so we can not hope for a good approximation to the energy eigenvalues if we completely ignore this interaction. One possibility is to try to find some function $U(r_i)$ containing the central part of $\Sigma \frac{1}{r_{ij}}$ and solve the eigenvalue problem for the central field Hamiltonian

$$H_{CF} = \sum_i \left(\frac{\underset{\sim}{p}_i^2}{2} - U(r_i)\right) \tag{1.4}$$

treating remaining terms

$$\sum_i \left(U(r_i) - \frac{z}{r_i}\right) + \sum_{i<j} \frac{1}{r_{ij}} \tag{1.5}$$

which hopefully will be small, by means of perturbation theory.

The Hartree-Fock unrestricted consistent field method determines a numerical radial function which on taking the spherical average of $\Sigma \frac{1}{r_{ij}}$ gives a minimum in the average energy of each electron[7,11]. Non-analytic methods, despite the better zero-order energies, make perturbation calculations messy with numerical integrations. Analytic forms we shall use for $U(r_i)$ make perturbation calculations simpler, but the corrections are larger.

Equation (1.3) is solved by putting

$$\Psi = \prod_i \psi_i$$
$$E_{CF} = \sum_i \varepsilon_i \qquad (1.6)$$

obtaining the uncoupled equations

$$(\frac{p_j^2}{2} - U(r_j))\psi_j = \varepsilon_j\psi_j \,. \qquad j = 1,2 \ldots N \qquad (1.7)$$

Function ψ_j is the eigenfunction for particle j moving in central field $U(r_j)$ and ε_j is the associated energy eigenvalue.

Electron spin is taken into account by multiplying ψ_j by the appropriate spin function α or β corresponding to the two allowed spin orientations $m_s = \pm\frac{1}{2}$ along the z-axis.

Any permutation of electron labels is also a solution to the central field problem, making the general solution a linear sum over all such permutations. To satisfy Pauli's exclusion principle we demand that the linear combination be antisymmetric, being readily achieved by constructing Slater determinants[6,11] from the single particle wavefunctions $\psi_j\{^{\alpha}_{\beta}\}$.

1.4 THE HYDROGENIC APPROXIMATION

Taking the central field to be the potential electron i sees from nuclear charge Z, equation (1.4) becomes

$$H_{CF} = \sum_i (\frac{p_i^2}{2} - \frac{Z}{r_i}) \qquad (1.8)$$

which is the sum of N hydrogen like Hamiltonians for nuclear charge Z. Hence the single particle wavefunctions are hydrogenic and uniquely specified by the four quantum numbers

$$n, \quad \ell = 0,1\ldots(n-1), \quad m_\ell = 0,\pm1,\ldots\pm\ell, \quad m_s = \pm\tfrac{1}{2}$$

where n is the principal quantum number and must be a positive integer, ℓ is the orbital angular momentum quantum number, m_ℓ the z-component of ℓ, and m_s the spin z-component.

Single particle energies are

$$\varepsilon_j = -\frac{Z^2}{2n_j^2} \tag{1.9}$$

The N-electron wavefunction is now specified by listing $n\ell m_\ell m_s$ for each electron, or by using a coupled representation in terms of total angular momenta. In Russell-Saunders coupling, all the ℓ and the s are coupled giving totals LS with total z-components M_L M_S respectively[6,11-13]. This scheme is suited to the non-relativistic problem since the Hamiltonian commutes with both S and L.

We shall use the standard convention of listing the $(n\ell)$ values in order of increasing n, and for constant n in increasing ℓ. If there are x electrons with the same $n\ell$ quantum numbers we write $n\ell^x$ instead of listing the $n\ell$ values x times.

Quantum numbers $n\ell$ specify the electrons orbital, n specifying the shell. From Pauli's exclusion principle there can be no more than $2(2\ell+1)$ electrons in orbital $n\ell$. An orbital, or shell, containing its maximum number of electrons is said to be full or closed. Electrons in the same orbital are equivalent as we cannot distinguish between them.

The collection of all $n\ell$ quantum numbers $(n\ell)$ is called a configuration. We shall use notation ℓ^N for a configuration in which there are N electrons in orbital ℓ (suppressing the principal quantum number), and all orbitals below ℓ in the conventional ordering are full. If an orbital below ℓ is

also open it shall be explicitly shown. The term core electrons is used for all full orbitals, and deep core for all full shells.

Parity of configuration $(n\ell)$ is[6]

$$p = (-1)^{\sum_i \ell_i}$$

so is either positive or negative. Positive parity is often referred to as even, and negative as odd.

The energy of an electron depends only on the shell it occupies, hence the total energy of a N-electron wavefunction in the hydrogenic approximation depends on the set of principal quantum numbers

$$(n) = n_1 n_2 \ldots n_N$$

This set, and the parity defines a complex $|(n)p\rangle$. All configurations in a complex have the same zero-order energy and are coupled by the remaining terms of the exact Hamiltonian.

1.5 RAYLEIGH-SCHRÖDINGER PERTURBATION THEORY

Details of Rayleigh-Schrödinger perturbation theory are treated in most quantum mechanics texts[6,11,14] so we shall only outline the results needed later.

Suppose Hamiltonian H can be written as

$$H = H_0 + \lambda V$$

such that the 'zero-order' eigenvalue problem

$$H_0|m\rangle = E_m^{(0)}|m\rangle$$

is solvable. We want to solve the complete eigenvalue problem

$$H|\Psi_m\rangle = E_m|\Psi_m\rangle$$

which we assume has solutions such that as λ tends to zero $|\Psi_m\rangle$ tends to $|m\rangle$ and E_m tends to $E_m^{(0)}$, i.e. that $|\Psi_m\rangle$ and E_m are analytic functions of λ and regular at $\lambda = 0$. If this is the case, there exist series expansions

$$|\Psi_m\rangle = \sum_{n=0}^{\infty} E_m^{(0)} |\Psi_m^{(n)}\rangle, \qquad |\Psi_m^{(0)}\rangle \equiv |m\rangle$$

$$E_m = \sum_{n=0}^{\infty} \lambda^n E_m^{(n)}$$

The first term in the energy expansion is the zero-order energy. The next three terms are

$$\begin{aligned} E_m^{(1)} &= \langle m|V|m\rangle \\ E_m^{(2)} &= \sum_t{}' \frac{\langle m|V|t\rangle\langle t|V|m\rangle}{(E_m^{(0)} - E_t^{(0)})} \\ E_m^{(3)} &= \sum_{st}{}' \frac{\langle m|V|s\rangle\langle s|V|t\rangle\langle t|V|m\rangle}{(E_m^{(0)}-E_s^{(0)})(E_m^{(0)}-E_t^{(0)})} \\ &\quad - \sum_t{}' \frac{\langle m|V|t\rangle\langle t|V|m\rangle\langle m|V|m\rangle}{(E_m^{(0)} - E_t^{(0)})^2} \end{aligned} \tag{1.10}$$

the primes indicating that the sums exclude states labelled by m.

If the zero-order wavefunctions are degenerate, expressions (1.10) must be diagonalized in the space of degenerate functions $|m\rangle$.

1.6 OPERATOR PERTURBATION THEORY

An alternative formalism of perturbation theory[15,16] is to define a unitary operator e^S with the property (using the

$$|\Psi_m\rangle = e^{-S}|m\rangle$$

and

$$\tilde{H} = e^{S} H e^{-S}$$

such that $\tilde{H}$ is diagonal in the representation based on the zero-order eigenfunctions, making

$$[\tilde{H},H_0] = 0$$

Now write

$$S = \sum_{n=1}^{\infty} \lambda^n S_n$$

No term independent of λ is included as we are demanding that $|\Psi_m\rangle$ tends to $|m\rangle$ as λ tends to zero.

The level-shift operator is defined as

$$\omega = \tilde{H} - H_0$$

such that

$$\omega|m\rangle = (E_m - E_m^{(0)})|m\rangle$$

Assuming we can write

$$\omega = \sum_{i=1}^{\infty} \lambda^i \omega_i$$

and using the Hausdorff formula we get

$$\omega = \lambda V + [S,H] + \frac{1}{2!}[S,[S,H]]$$

Equating coefficients of λ when the series forms for S and ω are substituted gives

$$\omega_1 = V + [S_1,H_0]$$

$$\omega_2 = [S_1,V] + [S_2,H] + \frac{1}{2!}[S_1,[S_1,H_0]]$$

Using that ω, hence $\omega_1, \omega_2 \ldots$, is diagonal in the representation in which H_0 is diagonal and the hyperviral theorem, stating that commutator $[H,Q]$ is off-diagonal in the representation in which H is diagonal, we obtain

$$\omega_1 = V^d, \qquad V^{od} = [H_0, S_1]$$

where V^d and V^{od} are the diagonal and off-diagonal parts of V respectively. A little manipulation gives

$$\omega_2 = -\tfrac{1}{2}[V^{od}, S_1]^d$$

By the definition of the level-shift operator the n^{th}-order correction to the zero-order eigenvalue $E_m^{(0)}$ is given by the matrix element of ω_n between the zero-order eigenfunctions.

1.7 PERTURBATION THEORY AND EFFECTIVE OPERATORS

Operator ω_n is an effective operator, the matrix elements in the space of zero-order functions giving the n^{th}-order correction to eigenvalue $E_n^{(0)}$. Equivalence between the two forms of perturbation will be shown in this section.

From operator perturbation theory

$$E_m^{(1)} = \langle m|\omega_1|m\rangle$$
$$= \langle m|V|m\rangle$$

Second order requires solving

$$V^{od} = [H_0, S_1]$$

for S_1. Following Primas[15]

$$S_1 = \sum_{m \neq n} \frac{P_m V^{od} P_n}{(E_m^{(0)} - E_n^{(0)})}$$

$|m\rangle$. This gives

$$\omega_2 = \sum_{n\neq m} \frac{(V^{od} P_n V^{od})^d}{(E_m^{(0)} - E_n^{(0)})}$$

so

$$E_m^{(2)} = \sum_n{}' \frac{\langle m|V|n\rangle\langle n|V|m\rangle}{(E_m^{(0)} - E_n^{(0)})}$$

The third order correction[16] from the operator formalism is

$$E_m^{(3)} = \sum_t{}' \frac{\langle m|V|t\rangle\langle t|V|m\rangle(\langle t|V|t\rangle - \langle m|V|m\rangle)}{(E_m^{(0)} - E_t^{(0)})^2}$$

$$+ \frac{1}{3} \sum_{t\neq s}{}' \left(\frac{1}{(E_t^{(0)} - E_s^{(0)})} + \frac{1}{(E_m^{(0)} - E_s^{(0)})}\right) \frac{1}{(E_m^{(0)} - E_t^{(0)})}$$

$$(\langle m|V|s\rangle\langle s|V|t\rangle\langle t|V|m\rangle + \langle m|V|t\rangle\langle t|V|s\rangle\langle s|V|m\rangle)$$

The connection between this result and the third-order Rayleigh-Schrödinger correction is best shown by means of diagrams[17].

That the linked-diagram theorem is associated with the unitary nature of operator e^S has been shown by Yaris and Musher[18]. This results in no unlinked diagrams in the operator formalism, whereas the Rayleigh-Schrödinger correction $E_m^{(3)}$ contains unlinked diagrams. By addition and subtraction of suitable terms both third order corrections are equivalent[18]. The same method will lead to equivalence to higher orders.

Increasing difficulty of obtaining higher order corrections makes it necessary to use other methods[19] but will not concern us.

Operator perturbation theory is closely related to Rajnak and Wybourne's[1-3] effective operator techniques. Their

effective operator, to a given order, is the level-shift operator to that order with the sum over intermediate states carried out for all intermediate quantum numbers associated with a given configuration.

1.8 THE Z-EXPANSION

It is shown in a later chapter that the Coulomb radial integrals for hydrogenic functions are proportional to Z, the nuclear charge. Since the zero-order energy is proportional to Z^2 the non-relativistic energy perturbation based on the hydrogenic approximation gives an expansion

$$E = E_0 Z^2 + E_1 Z + E_2 + E_3 Z^{-1} + \ldots \qquad (1.11)$$

coefficient E_n coming from n^{th}-order perturbation theory. If the ground complex contains more than one configuration, coefficients $E_1, E_2 \ldots$ are square matrices. The total energy is obtained on diagonalizing energy matrix

$$E_0 Z^2 + E_1 Z + E_2 + \ldots \qquad (1.12)$$

Energy matrix (1.12) must be diagonalized for each Z even though coefficients $E_0, E_1, \ldots$ are fixed for an isoelectronic sequence.

Expansion (1.11) leads directly to the generalized empirical law of Moseley stating that for a homologous series of atoms (atoms having equal numbers of electrons and which are in corresponding states) the ionization potential is proportional to Z^2. The screening doublet law, stating that the energy difference between two spectroscopic terms in the same configuration is proportional to Z along an isoelectronic

sequence, also follows[5]. Edlén[20] has used this expansion, with great success, showing trends in isoelectronic and homologous sequences.

Layzer[4] has shown that the rate of convergence for this expansion depends strongly on the degree of ionization and weakly on the number of electrons in the complex. If Z-N > 3 he has shown that E_3 is usually smaller than relativistic corrections.

Layzer[21] has made the very interesting point that relativistic level shifts in an isoelectronic sequence may be readily separated out from the non-relativistic energy contributions by their characteristic Z dependence. The difference

$$\Delta E = E_{exp} - E_0 Z^2 - E_1 Z$$

with E_{exp} being the experimental energy, is obtainable exactly since E_0 and E_1 are known for a given complex. Remaining non-relativistic contributions tend to the constant value of E_2 as Z increases, leaving the relativistic corrections.

Spin-orbit radial integrals, as shown later, are proportional to the fourth power of Z making the second-order spin-orbit-spin-orbit perturbation term proportional to Z^6, while the spin-orbit-Coulomb perturbation term is proportional to Z^3.

Layzer and Bahcall[22] have included the Breit interaction in their perturbation, resulting in the double power series in Z^{-1} and $\gamma = \alpha^2 Z^2$, α the fine structure constant,

$$E = Z^2 \sum_{ij=1}^{\infty} E_{ij} Z^{-i} \gamma^j \qquad (1.13)$$

This does not allow for the Lamb shift and other second order

relativistic interactions[23]. Helium and lithium sequences have been treated with success on including the first order relativistic correction in (1.13). Doyle's review article contains references to calculations of E_{00}, E_{10}, E_{20}, E_{01} and E_{11} for the He and Li. Neither of these sequences has a spin-orbit contribution but they do contain a Z^3 term.
Layzer[5] has shown how energy calculations can be improved without going to second-order perturbation theory. It involves screening parameters determined by first-order calculations. The zero-order energy is written as

$$E = \sum_{\alpha} \frac{q_\alpha (Z-S_\alpha)^2}{2n_\alpha^2}$$

$\alpha = 1,2,3...$ according to conventional ordering of orbitals $\alpha(1s) = 1$, $\alpha(2s) = 2$, $\alpha(2p) = 3$ ..., q_α is the number of electrons in orbital α, and S_α the screening parameter. This leads to an estimate of the third-order correction

$$E_2 \sim \sum_{\alpha} \frac{q_\alpha S_\alpha^2}{2n_\alpha^2}$$

from first-order calculations assuming nuclear charge Z for all orbitals. This method is extendable to relativistic corrections[23].

Hydrogen radial functions within a given shell have their principal maxima at about the same distance from the nucleus[24] resulting in screening parameters within a shell being approximately equal and increasing with n, as found by Layzer[5]. Consequently screened radial functions $R_{n\ell}(Z)$ and $R_{n',\ell}(Z')$ will not be orthogonal if Z and Z' differ, as they do in screening theory. Conventional perturbation theory cannot be used to

improve the zero-order energies as it is based on the assumption of basis states being orthogonal. An orthogonal basis set could be constructed using Schmidt's orthogonalization procedure[26] but then the concept of a complex is lost.

1.9 Z-EXPANSION FOR HARTREE-FOCK CALCULATIONS

The Hartree-Fock Z-expansion has been studied by numerous people[27-30]. Layzer[28] has shown that in the extended Hartree-Fock approximation (variational state functions are taken to be the same linear combination of single configurational state functions as in the hydrogenic approximation) the energy can be expanded according to equation (1.11) with E_0 and E_1 the same as in the hydrogenic approximation and E_2, the second-order perturbation correction, is obtained when intermediate configurations are restricted to involving single electron excitations, from the ground configurations, into orbitals with the same orbital quantum numbers as occupied in the ground complex. Also all other quantum numbers of both perturbed and perturbing configurations must be the same.

Stewart[29] and Coulson[30] have studied the Z-expansion in the unrestricted Hartree-Fock approximation and found that it involves half integer powers of Z as well as integer powers.

CHAPTER 2

DERIVATION OF SECOND-ORDER EFFECTIVE OPERATORS

2.1 INTRODUCTION

Firstly we define an effective operator which leads to the second-order effective operators needed for a perturbing potential expresses as a sum of the Coulomb repulsion and the spin-orbit interaction. The operators obtained by Rajnak and Wybourne are generalized to a non-Hartree-Fock central field. We also calculate the second-order scalar operators previously neglected. Having listed all allowed excitations we show by specific examples how effective operators may be calculated. A list of second-order effective operators, for our perturbing potential, and an open n = 2 shell, is found in Appendix A.

2.2 DEFINITION OF AN EFFECTIVE OPERATOR

In general, perturbation V will couple states of one complex with those of another complex. The second-order correction to the energy matrix of complex A, due to its interaction with complex B, is

$$\sum_{\beta} \frac{\langle A\alpha|V|B\beta\rangle\langle B\beta|V|A\alpha'\rangle}{(E_A - E_B)}$$

the sum being over all states $|B\beta\rangle$ of complex B, Greek letters representing remaining quantum numbers required to uniquely specify the state, and E_A is the energy of complex A. Alternatively this can be considered as the diagonalization of the operator

$$\theta = V + \sum_{\beta} \frac{V|B\beta\rangle\langle B\beta|V}{(E_A - E_B)} \qquad (2.1)$$

in complex A.

By means of operator θ the entire energy to second-order is found by considering matrix elements in complex A. We are no longer concerned with matrix elements other than those between states contained in complex A.

Since, from the definition of a complex, the energy denominator depends only on the complex and not quantum numbers β, we are interested in evaluating sums of the form

$$\sum_{\beta} V|B\beta\rangle\langle B\beta|V$$

extending to higher order corrections as

$$\sum_{\beta\gamma\ldots\omega} V|B\beta\rangle\langle B\beta|V|C\gamma\rangle\langle C\gamma|V \ \ldots\ V|Z\ddot{\omega}\rangle\langle Z\omega|V$$

We shall consider second-order corrections, but the methods are quite general.

If we could redefine V such that it gives a null result when acting on any complex other than B we could write

$$\sum_{\beta} V|B\beta\rangle\langle B\beta|V = \sum_{Z\omega} V(AB)\,|Z\omega\rangle\langle Z\omega|V(BA)$$

$$= V(AB)V(BA) \qquad (2.2)$$

where the sum is over all complexes and all states within the complex. Completeness of states $|Z\omega\rangle$ has been used in requiring[31]

$$\sum_{Z\omega} |Z\omega\rangle\langle Z\omega| \equiv 1$$

Operator V(AB) is defined such that it is identical to V when acting to the left of B and to the right of A, and is the null operator otherwise. The product operator $V(AB)V(BA)/(E_A-E_B)$ is the second-order effective operator for perturbation V and intermediate complex B.

We shall not be able to do the sum over all states contained in the excited complex, but only over states associated with a particular configuration of a complex. We can do summations over angular momenta variables by means of angular momentum theory, but summations over configurations still elude us and must be done numerically.

2.3 SECOND-ORDER EFFECTIVE OPERATORS

We are interested in the perturbation

$$V = \sum_{i<j} \frac{1}{r_{ij}} + \sum_{i} \zeta(r_i)\ (\underset{\sim}{s}^{(1)} . \underset{\sim}{\ell}^{(1)}) \qquad (2.3)$$

which to second-order gives rise to

i) Coulomb-Coulomb part only

ii) Spin-orbit-spin-orbit part only

iii) Coulomb-spin-orbit part only,

with the interaction name referring, in order, to the two operators in (2.2). Coulomb and spin-orbit operators being Hermitian makes the Coulomb-spin-orbit and spin-orbit-Coulomb product operators equal when the bra and ket is for the same configuration, this does not hold for off-diagonal effective operators.

We shall consider each case separately.

2.4 POSSIBLE EXCITATIONS INDUCED BY A TWO PARTICLE OPERATOR FROM GROUND CONFIGURATIONS ℓ^N AND $\ell'^4\ell'\ell^{N+2}$

Firstly consider configuration ℓ^N. The entire set of allowed excitations by a two-particle operator is shown in Table I. Excitations *(a)*, *(b)* and *(c)* involve promotion of two electrons from the same core orbital, in case *(a)* they both go into empty orbitals, in case *(b)* one goes into the open orbital and the other into an empty orbital, while in case *(c)* both go

TABLE I

Allowed Excitations from ℓ^N by a Two-Particle Operator

(a) $\ell'^{4\ell'}\ell^N\ell''^2$, $\ell'^{4\ell'}\ell^N\ell''\ell'''$

(b) $\ell'^{4\ell'}\ell^{N+1}\ell''$

(c) $\ell'^{4\ell'}\ell^{N+2}$

(d) $\ell'^{4\ell'+1}\ell''^{4\ell''+1}\ell^N\ell'''^2$, $\ell'^{4\ell'+1}\ell''^{4\ell''+1}\ell^N\ell'''\ell''''$

(e) $\ell'^{4\ell'+1}\ell''^{4\ell''+1}\ell^{N+1}\ell'''$

(f) $\ell'^{4\ell'+1}\ell''^{4\ell''+1}\ell^{N+2}$

(g) $\ell^{N-2}\ell'^2$, $\ell^{N-2}\ell'\ell''$

(h) $\ell'^{4\ell'+1}\ell^{N-1}\ell''^2$, $\ell'^{4\ell'+1}\ell^{N-1}\ell''\ell'''$

(i) $\ell^{N-1}\ell'$

(j) $\ell'^{4\ell'+1}\ell^N\ell''$

(k) $\ell'^{4\ell'+1}\ell^{N+1}$

into the open orbital. Excitations *(d)*, *(e)* and *(f)* again involve two core electrons, this time from different orbitals. Case *(h)* involves excitation of one core and one open orbital electron. Cases *(i)*, *(j)* and *(k)* are the three possible single particle excitations.

A particular case may not allow all listed excitations. If N = 4ℓ+1 cases *(c)* and *(f)* are forbidden, if N = 1 case *(g)* is forbidden. Parity conservation will further limit allowed excitations.

Configuration $\ell'^{4}\ell'\ell^{N+2}$ is contained in the same complex as ℓ^N if orbitals ℓ and ℓ' are in the same shell. These are the only configurations in the complex if the open shell has principal quantum number two, forcing ℓ' to be a s-orbital. We shall consider this case.

The set of allowed excitations, assuming ℓ' is an s-orbital, is shown in Table II.

Orbital ℓ' being initially empty puts this orbital into the same category as the empty orbitals above ℓ, hence no new effective operators are needed.

With more than one configuration in the ground complex, interconfigurational excitations must also be considered. The set of intermediate configurations which permit such interactions, off-diagonal in configurational space, are shown in Table III.

Case *(b)* is most easily evaluated by conventional means so the corresponding effective operator has not been calculated. In the special case of an open shell with principal quantum number two case *(e)* does not conserve parity and will therefore be ignored.

TABLE II

Allowed Excitations from $\ell'^{4\ell'}\ell^{N+2}$ by a Two-Particle Operator, if ℓ' is an s-orbital

(a) $\ell'^{4\ell'+1}\ell^{N}\ell''$

(b) $\ell'^{4\ell'}\ell^{N}\ell''^{2}$, $\ell'^{4\ell'}\ell^{N}\ell''\ell'''$

(c) $\ell_1^{4\ell_1}\ell^{N+2}$

(d) $\ell_1^{4\ell_1}\ell^{4\ell'+1}\ell^{N+3}$

(e) $\ell_1^{4\ell_1}\ell'^{4\ell'+1}\ell^{N+2}\ell''$

(f) $\ell_1^{4\ell_1}\ell^{4\ell'}\ell^{N+4}$

(g) $\ell_1^{4\ell_1}\ell'^{4\ell'}\ell^{N+3}\ell''$

(h) $\ell_1^{4\ell_1}\ell'^{4\ell'}\ell^{N+2}\ell''^{2}$, $\ell_1^{4\ell_1}\ell'^{4\ell'}\ell^{N+2}\ell''\ell'''$

(i) $\ell'^{4\ell'+1}\ell^{N+1}$

(j) $\ell'^{4\ell'}\ell^{N+1}\ell''$

(k) $\ell_1^{4\ell_1+1}\ell'^{4\ell'+1}\ell^{N+2}$

(l) $\ell_1^{4\ell_1+1}\ell'^{4\ell'}\ell^{N+3}$

(m) $\ell_1^{4\ell_1+1}\ell'^{4\ell'}\ell^{N+2}\ell''$

TABLE III

Allowed Excitations by a Two-Particle Operator giving rise to Off-diagonal Interactions between Ground Configurations ℓ^N and $\ell'^{4\ell'}\ell^{N+2}$

(a) $\ell'^{4\ell'}\ell^N\ell''^2$, $\ell'^{4\ell'}\ell^N\ell''\ell'''$

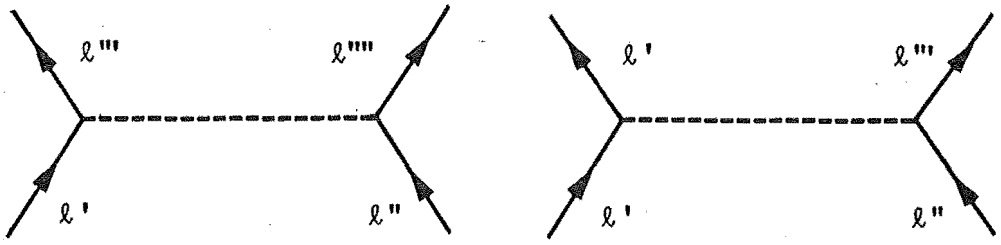
(b) $\ell_1^{4\ell_1}\ell^{N+2}$

(c) $\ell'^{4\ell'}\ell^{N+1}\ell''$

(d) $\ell'^{4\ell'+1}\ell^N\ell''$

(e) $\ell'^{4\ell'+1}\ell^{N+1}$

Excitations produced by a two particle operator have interaction diagrams



(i) (ii)

Diagram (i) refers to a two electron excitation with electrons initially in orbitals ℓ' and ℓ'' being promoted into orbitals ℓ''' and ℓ''''. Since both electrons are in different orbitals after the interaction these are referred to as 'active'. Diagram (ii) is a single electron excitation and since the electron in orbital ℓ' remains in this orbital it is called 'passive'. In a single particle excitation, the passive electron can come from any of the occupied orbitals. We shall use the notation ℓ_1, or ℓ_2, for such a passive electron coming from an orbital not explicitly shown in the intermediate configuration. A sum over such orbitals is assumed.

2.5 RESTRICTION ON POSSIBLE EXCITATIONS FOR A HARTREE-FOCK CENTRAL FIELD

If the central field is[32,33]

$$U = \sum_{\alpha\alpha'} |\alpha\rangle\langle\alpha'| \ \langle\alpha|U|\alpha'\rangle$$

with

$$\langle\alpha|U|\alpha'\rangle = \sum_{\beta} \frac{N\beta}{2(2\ell_\beta+1)}\{\langle\alpha_1\beta_2|\frac{1}{r_{12}}|\alpha_1\beta_2\rangle - \langle\alpha_1\beta_2|\frac{1}{r_{12}}|\beta_1\alpha_2\rangle\}$$

α,α' and β being single electron states, β an orbital from the ground configuration, $N\beta$ the occupation number of orbital β, then there are no perturbation contributions from one-electron excitations due to interactions involving passive orbitals closed in the ground configuration. The closed orbital Hartree-Fock potential is U, so in this approximation we need not consider passive excitations involving orbitals which are closed in the ground configuration.

Rajnak and Wybourne[9] and later Racah and Stein[34] in their calculation of effective operators have ignored passive excitations from orbitals closed in the ground configuration except in the case of intermediate configuration $\ell'^{4\ell'+1}\ell^{N+1}$. We shall include such passive excitations making our effective operators more general.

Since we are interested in obtaining Layzer's energy Z-expansion we use the central field $-\Sigma \frac{Z}{r_i}$ and not the better zero-order Hartree-Fock potential.

2.6 COULOMB-COULOMB EFFECTIVE OPERATORS

By virtue of the spherical-harmonic addition theorem the Coulomb interaction, in tensorial form, is[13]

$$\sum_{i<j} \frac{1}{r_{ij}} = \sum_{k} \sum_{i<j} \frac{r_<^k}{r_>^{k+1}} (\underset{\sim}{C}_i^{(k)} . \underset{\sim}{C}_j^{(k)}) \qquad (2.4)$$

where $\underset{\sim}{C}^{(k)}$ is the tensorial form of the spherical-harmonics, $r_<$ the lesser and $r_>$ the greater of r_i and r_j. We shall use Judd's[13] definition of the scalar product

$$(\underset{\sim}{T}^{(k)} . \underset{\sim}{U}^{(k)}) = \sum_{q} (-)^q T_q^{(k)} U_{-q}^{(k)}$$

differing from that of Fano and Racah[35] by the phase $(-)^q$.

In the central field approximation zero-order wavefunctions are separable into radial and angular parts, matrix elements in this representation factorizing in the same way[6]. The general matrix elements of the Coulomb operator are expressible as a linear sum over two-particle matrix elements

$$\langle ab|\frac{1}{r_{ij}}|cd\rangle = \sum_{k} R^k(ab,cd) \langle ab|(\underset{\sim}{C}_i^{(k)} . \underset{\sim}{C}_j^{(k)})|cd\rangle$$

with

$$R^k(ab,cd) = \int_0^\infty \int_0^\infty \frac{r_<^k}{r_>^{k+1}} R_a(r_1) R_b(r_2) R_c(r_1) R_d(r_2) r_1^2 r_2^2 dr_1 dr_2 \qquad (2.5)$$

The angular part can be evaluated by the methods of coupled states[13] or determinantal states[6].

It is convenient to work with unit tensor operators whose single particle reduced matrix elements are unity. Elliott[36] has defined unit orbital tensor operator $\underset{\sim}{u}^{(k)}(n\ell,n'\ell')$ for mixed configurations as

$$\langle n\ell \,||u^{(k)}(n'\ell',n''\ell'')||\, n'''\ell'''\rangle = \delta(nn')\delta(n''n''')\,\delta(\ell\ell')\delta(\ell''\ell''')$$

The more general unit operator is one acting in both spin and orbital spaces, defined as

$$\langle s\ell \,||u^{(kk')}(s'\ell',s''\ell'')||\, s'''\ell'''\rangle = \delta(ss')\delta(s''s''')\delta(\ell\ell')\delta(\ell''\ell''')$$

the principal quantum numbers being suppressed as shall be done from now on, and k being the rank in spin space and k' rank in orbital space.

For a configuration containing N electrons one defines operators

$$\underset{\sim}{U}^{(k)}(\ell\ell') = \sum_{i=1}^{N} \underset{\sim i}{u}^{(k)}(\ell\ell')$$

and

$$\underset{\sim}{U}^{(kk')}(s\ell,s'\ell') = \sum_{i=1}^{N} \underset{\sim i}{u}^{(kk')}(s\ell,s'\ell')$$

Note that these definitions do not contain normalizations $(2k+1)^{\frac{1}{2}}$ and $\{(2k+1)(2k'+1)\}^{\frac{1}{2}}$ of Judd's $\underset{\sim}{v}^{(k)}$ and $\underset{\sim}{w}^{(kk')}$ respectively. No confusion results from using symbol u for both of these operators since the first has a single rank while the second has a double rank.

Consider perturbing configuration $\ell^{N-2}\ell'^{2}$. The second-order correction is

$$\sum_{\beta} \langle \ell^N \gamma SL | \sum_{i<j} \frac{1}{r_{ij}} | \ell^{N-2}\ell'^{2}\beta SL\rangle \langle \ell^{N-2}\ell'^{2}\beta SL | \sum_{p<q} \frac{1}{r_{pq}} | \ell^N \gamma' SL\rangle / \Delta E \qquad (2.6)$$

In this case

$$\sum_{i<j} \frac{1}{r_{ij}} = \sum_{k} \langle \ell \| C^{(k)} \| \ell' \rangle^2 R^k(\ell\ell,\ell'\ell') \sum_{i<j} (\underset{\sim i}{u}^{(k)}(\ell\ell') . \underset{\sim j}{u}^{(k)}(\ell\ell')) \qquad (2.7)$$

With this form of the Coulomb operator the sum over β in equation (2.6) can be replaced by a complete set of states.

Introduce the notation of Rajnak and Wybourne[1]

$$X(k,\ell_a\ell_b\ell_c\ell_d) = \langle \ell_a \| C^{(k)} \| \ell_c \rangle \langle \ell_b \| C^{(k)} \| \ell_d \rangle R^k(ab,cd)/\Delta E^{\frac{1}{2}}$$

$$P(kk',\ell_a\ell_b\ell_c\ell_d) = X(k,\ell_a\ell_b\ell_c\ell_d) X(k',\ell_a\ell_b\ell_c\ell_d)$$

$$M(k,\ell_a\ell_b\ell_c\ell_d) = \sum_{kk'} \begin{Bmatrix} k & k' & t \\ \ell_a & \ell_b & \ell_c \end{Bmatrix} \begin{Bmatrix} k & k' & t \\ \ell_a & \ell_b & \ell_d \end{Bmatrix} P(kk',\ell_a\ell_b\ell_c\ell_d)$$

We have put the positive square root of the energy denominator in the definition of X and not ΔE with P as the product of two Xs is more general than the earlier definition of P.

Now the effective operator can be written as

$$\sum_{kk'} P(kk',\ell\ell\ell'\ell') \sum_{\substack{i<j \\ p<q}} (\underset{\sim}{u}_i^{(k)}(\ell\ell').\underset{\sim}{u}_j^{(k)}(\ell\ell'))(\underset{\sim}{u}_p^{(k')}(\ell'\ell).\underset{\sim}{u}_q^{(k')}(\ell'\ell))$$

Operator $(\underset{\sim}{u}_i^{(k)}(\ell\ell').\underset{\sim}{u}_j^{(k)}(\ell\ell'))$ acts only on a state where electrons i and j are in orbital ℓ', and since configuration ℓ^N has an empty ℓ' orbital we obtain a non-zero contribution only if operator $(\underset{\sim}{u}_p^{(k')}(\ell'\ell).\underset{\sim}{u}_q^{(k')}(\ell'\ell))$ has put electrons i and j into orbital ℓ'. Hence i = j, p = q are the only contributors. The product operator

$$\sum_{i<j} (\underset{\sim}{u}_i^{(k)}(\ell\ell').\underset{\sim}{u}_j^{(k)}(\ell\ell'))(\underset{\sim}{u}_i^{(k')}(\ell'\ell).\underset{\sim}{u}_j^{(k')}(\ell'\ell))$$

is rearranged using recoupling theory[12,13,35]. One finally ends up with the simplified operator

$$\sum_{k} (-)^k[k]M(k,\ell\ell\ell'\ell') \sum_{i<j} (\underset{\sim}{u}_i^{(k)}.\underset{\sim}{u}_j^{(k)})$$

with the unit operators acting in orbital ℓ only. We suppress the orbitals in the tensor operators when they act solely in orbital ℓ. Standard notation

$$[k] = 2k + 1$$

has been used.

The difference between our effective operator and that of Racah and Stein[34] is in our different definitions of the scalar product.

In the more general case we obtain product operator

$$\sum_{i\neq j} (\underset{\sim}{u}_i^{(k)}(\ell'\ell''').\underset{\sim}{u}_j^{(k)}(\ell''\ell'''')) (\underset{\sim}{u}_i^{(k')}(\ell'''\ell').\underset{\sim}{u}_j^{(k')}(\ell''''\ell''))$$

which on recoupling gives a product of operators acting on the same electron simplified by using

$$\{\underset{\sim}{u}_i^{(k)}(\ell\ell') \times \underset{\sim}{u}_i^{(k')}(\ell'\ell''')\}^{k''} = (-)^{\ell+\ell'''+k''}[k'']^{\frac{1}{2}} \begin{Bmatrix} k & k' & k'' \\ \ell''' & \ell & \ell' \end{Bmatrix} \underset{\sim}{u}_i^{(k'')}(\ell\ell''')$$

giving

$$\sum_{k''} \sum_{i\neq j} \{\underset{\sim}{u}_i^{(k'')}(\ell'\ell') \times \underset{\sim}{u}_j^{(k'')}(\ell''\ell'')\}_0^0$$

Orbitals ℓ' and ℓ'' may be full or the open orbital ℓ. If orbital ℓ' is full, then

$$\langle \ell^N | U^{(k'')}(\ell'\ell') | \ell^N \rangle = \delta(k''0)\ 2[\ell']^{\frac{1}{2}}$$

and if $\ell'' \equiv \ell$

$$\langle \ell^N | U^{(0)} | \ell^N \rangle = N/[\ell]^{\frac{1}{2}}.$$

A detailed account of recoupling formulae needed has been given by Wybourne[3].

A list of the effective operators needed for the ground complex containing configurations ℓ^N and $\ell'^{4\ell'}\ell^{N+2}$, with open shell n = 2, is contained in Appendix A.

The effective operators for ground configuration $\ell'^{4\ell'}\ell^{N+2}$, with ℓ' a s-orbital, for intermediate configurations listed in Table II are the same as for ground configuration ℓ^N. Correspondence between excitation species in Tables I and II is found by noting that orbital ℓ' in configuration $\ell'^{4\ell'}\ell^{N+2}$ is empty. Interactions, off-diagonal in configurational space, listed in Table III are treated in the same way as diagonal

interactions, with both ℓ' and ℓ orbitals being open in configuration $\ell'^{4\ell'}\ell^{N+2}$. The off-diagonal effective operators will be found in Appendix A except for case *(b)* which is easiest treated by conventional methods and case *(e)* which does not arise for reasons stated earlier.

Briggs[37] has extended Yutsis *et al.*[12] diagramatic methods to the evaluation of matrix elements for many electron wave-functions, which is essentially the same method as we are using with the coupled representation. Few identities from recoupling theory are needed, so there would be no advantage in using the diagrammatic methods.

2.7 EFFECTIVE OPERATORS VIA SECOND QUANTIZATION

Another approach to effective operators is to work with uncoupled states. Writing the operator and states in second quantization form[32], and rearranging the annihilation creation operator product to bring all the creation operators acting in full shells to the right, as such operators acting on $|\ell^N\rangle$ give a null result, leaves a sum of delta functions multiplied by two matrix elements, and 3-j symbols, as well as in some cases operators acting in the open orbital. Summing over all $m_s m_\ell$ values for each electron the 6-j symbols obtained by the previous method result.

This second quantization approach is inferior to that of the unit operators since the level of summations is lower leading to tedious rearrangements and summations taken care of in the coupled scheme by coupling theory.

Judd has shown[32] that unit operators can be represented as a coupled product of a creation-annihilation operator pair.

$$u_q^{(k)}(\ell\ell') = -\sum_{\zeta\eta} \langle \ell m_{\ell\zeta}, \ell' m_{\ell\eta} | \ell\ell'; kq \rangle a_\zeta^\dagger b_\eta$$

where $a^\dagger$ and b act in orbitals ℓ and ℓ' respectively. We could equally well work with coupled creation-annihilation operators as with unit operators $\underset{\sim}{u}^{(k)}$.

2.8 POSSIBLE EXCITATIONS INDUCED BY A ONE-PARTICLE OPERATOR, DIAGONAL IN ℓ, FROM GROUND CONFIGURATIONS ℓ^N AND $\ell'^{4\ell'}\ell^{N+2}$

The only single particle perturbation operator we shall be concerned with is the spin-orbit interaction which is diagonal in ℓ [6].

Possible excitations from configuration ℓ^N by the spin-orbit operator are listed in Table IV. The principal quantum number is explicitly shown since the diagonality in the orbital quantum number demanded can then be shown.

TABLE IV

Allowed Excitations from ℓ^N by the Spin-Orbit Operator

(a) $n\ell^{N-1}n'\ell$

(b) $n'\ell^{4\ell+1}n\ell^{N+1}$

(c) $n'\ell'^{4\ell'+1}n\ell^N n''\ell'$

As explained earlier, we are assuming that the open shell corresponds to a principal quantum number of two. Hence only excitation *(a)* gives a non-zero spin-orbit contribution.

Spin-orbit excitations from configuration $\ell'^{4\ell'}\ell^{N+2}$ are similar to those in Table IV.

2.9 SPIN-ORBIT-SPIN-ORBIT EFFECTIVE OPERATORS

We shall only consider case *(a)* of Table IV.

In atomic units the spin-orbit operator is

$$\frac{1}{2c^2} \sum_i \frac{1}{r_i} \frac{\partial U}{\partial r_i} \left(\underset{\sim}{s}_i^{(1)} . \underset{\sim}{\ell}_i^{(1)}\right)$$

which in the hydrogenic approximation reduces to

$$\frac{Z}{2c^2} \sum_i \frac{1}{r_i^3} \left(\underset{\sim}{s}_i^{(1)} . \underset{\sim}{\ell}_i^{(1)}\right)$$

as the central field is $U(r_i)$ the potential electron i sees from nuclear charge Z.

Reduced matrix elements of the spin and orbital operators are[13]

$$\langle s \,||s^{(1)}|| \, s\rangle = \{s(s+1)(2s+1)\}^{\frac{1}{2}} = (3/2)^{\frac{1}{2}}$$

$$\langle \ell \,||\ell^{(1)}|| \, \ell\rangle = \{\ell(\ell+1)(2\ell+1)\}^{\frac{1}{2}}$$

The spin-orbit operator in terms of unit operators is therefore

$$\frac{Z}{2c^2} \left\{\frac{3}{2} \ell(\ell+1)(2\ell+1)\right\}^{\frac{1}{2}} \sum_i \frac{1}{r_i^3} \left(\underset{\sim}{t}_i^{(1)} . \underset{\sim}{u}_i^{(1)}\right),$$

$\underset{\sim}{t}^{(1)}$ being a unit operator acting in spin space only while $\underset{\sim}{u}^{(1)}$ acts in orbital space. We can write

$$\{\underset{\sim}{t}_i^{(1)} . \underset{\sim}{u}_i^{(1)}\}^0 = \underset{\sim}{u}_i^{(11)0}$$

superscript zero indicating that the two unit ranks have been coupled up to give zero total rank.

Spin-orbit-spin-orbit effective operator for case *(a)* is

$$\frac{3}{2} \ell(\ell+1)(2\ell+1) \frac{\zeta^2_{n\ell,n'\ell}}{\Delta E} \cdot 3 \sum_{ij} \underset{\sim}{u}_i^{(11)0}(s\ell,s'\ell') \underset{\sim}{u}_j^{(11)0}(s'\ell',s\ell),$$

spin-orbit radial integral $\zeta_{n\ell,n'\ell}$ being defined as

$$\zeta_{n\ell,n'\ell} = \frac{Z}{2c^2} \int_0^\infty \frac{1}{r^3} R_{n\ell}(r) R_{n'\ell}(r) r^2 dr \qquad (2.10)$$

Using the same techniques as earlier we derive the result

$$\sum_i \underset{\sim i}{u}^{(11)0}(s\ell,s'\ell') \; \underset{\sim i}{u}^{(11)0}(s'\ell',s\ell)$$

$$= \sum_k (-)^{k+1}[k] \begin{Bmatrix} 1 & 1 & k \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{Bmatrix} \begin{Bmatrix} 1 & 1 & k \\ \ell & \ell & \ell \end{Bmatrix} \sum_i \underset{\sim i}{u}^{(kk)0}(s\ell,s\ell)$$

giving the spin-orbit-spin-orbit effective operator

$$\frac{\zeta^2_{n\ell,n'\ell}}{2\Delta E} \left\{ \frac{N\ell(\ell+1)}{2} - \sum_i (\underset{\sim i}{s}^{(1)} . \underset{\sim i}{\ell}^{(1)}) \right\}$$

For brevity of notation we shall include the positive square root of ΔE in the spin-orbit radial integral.

This result agrees with that of Rajnak and Wybourne[2] obtained by doing summations involving coefficients of fractional parentage.

In the special case being considered of orbital ℓ' in configuration $\ell'^{4}\ell'\ell^{N+2}$, there are no off-diagonal contributions from the spin-orbit-spin-orbit interaction.

2.10 COULOMB-SPIN-ORBIT EFFECTIVE OPERATORS

Noting that

$$\underset{\sim i}{u}^{(0k)} = \underset{\sim i}{u}^{(k)}$$

we can easily write the effective operator for the Coulomb-spin-orbit interaction for case *(a)* in terms of double tensor operators, the Coulomb part containing passive electrons.

After rearrangement the result given in Appendix A is obtained, agreeing with Rajnak and Wybourne for the terms in

which the passive electron comes from open orbital ℓ.

This interaction permits an off-diagonal contribution for intermediate configuration $\ell'^{4\ell'}\ell^{N+1}\ell''$ where the Coulomb operator excites two electrons from orbital ℓ' into ℓ and ℓ'', the spin-orbit operator demoting the ℓ'' electron into orbital ℓ. There is no non-zero spin-orbit-Coulomb off-diagonal interaction. The corresponding effective operator is given in Appendix A.

2.11 HIGHER ORDER PERTURBATIONS

The method outlined for obtaining second-order effective operators for a perturbation consisting of the Coulomb repulsion and the spin-orbit operator is readily applied to higher order corrections and to other interactions expressible in terms of tensor operators. Higher order effective operators for one particle excitations will be very lengthy as the number of terms involving passive electrons quickly grows. If we can assume a Hartree-Fock central field then higher orders could be handled without obtaining an unreasonable number of terms.

The number of different effective operators needed quickly grows with the order, but the major contributions could be obtained by considering a small number of the possible intermediate configurations.

Wybourne[3] has looked at a few third-order effective operators to find what new angular dependence results when higher order effects are considered. He shows that selection rules valid to second-order may be broken in third-order leading to an experimental way of finding the importance of such higher order contributions.

CHAPTER 3

EVALUATION OF ANGULAR MATRIX ELEMENTS

3.1 INTRODUCTION

The last two chapters have shown that configurational mixing can be entirely taken into account by operators acting in the space of degenerate zero-order wavefunctions. This is one big advantage of the effective operator formalism, resulting in only the coefficients of fraction parentage (cfp) for the open orbitals being needed. Difficulties of phases and normalizations associated with the more complicated cfp's do not arise[38]. Furthermore, the dimension of the energy matrix to be diagonalized is small being the number of degenerate ground states in the ground complex.

Since we are concerned with second-order theory we must evaluate reduced matrix elements of three coupled unit operators at the most.

A two-particle n^{th}-order perturbation effective operator, diagonal in the configuration, will contain at the highest a (n+1)-particle operator.

Angular momentum theory being well understood makes evaluation of angular matrix operators a process of substituting into standard formulae.

3.1 SYMMETRIC FORMS FOR TWO- AND THREE-PARTICLE OPERATORS ACTING IN A SINGLE ORBITAL

Many of the second-order effective operators for a two-particle perturbation

$$\sum_{i \neq j} g(i,j)$$

involve angular operators of the forms

$$\sum_{ij}{}' (\underset{\sim}{u}_i^{(k)} . \underset{\sim}{u}_j^{(k)}) = \sum_{i \neq j} (\underset{\sim}{u}_i^{(k)} . \underset{\sim}{u}_j^{(k)})$$

$$\sum_{pqr}{}' (\underset{\sim}{u}_p^{(k)} . \underset{\sim}{u}_q^{(k')} . \underset{\sim}{u}_r^{(k")}) = \sum_{\substack{p \neq q \\ p \neq r \\ q \neq r}} (\underset{\sim}{u}_p^{(k)} . \underset{\sim}{u}_q^{(k')} . \underset{\sim}{u}_r^{(k")})$$

For evaluation of the matrix elements it is more convenient to work with the operators $\underset{\sim}{U}^{(k)}$ defined earlier.

We have that

$$(\underset{\sim}{U}^{(k)} . \underset{\sim}{U}^{(k)}) \equiv \sum_{ij} (\underset{\sim}{u}_i^{(k)} . \underset{\sim}{u}_j^{(k)})$$

$$= \sum_{ij}{}' (\underset{\sim}{u}_i^{(k)} . \underset{\sim}{u}_j^{(k)}) + \frac{N}{[\ell]}$$

and

$$(\underset{\sim}{U}^{(k)} . \underset{\sim}{U}^{(k')} . \underset{\sim}{U}^{(k")}) = \sum_{pqr}{}' (\underset{\sim}{u}_p^{(k)} . \underset{\sim}{u}_q^{(k')} . \underset{\sim}{u}_r^{(k")})$$

$$+ (-)^{k+k'+k"} \begin{Bmatrix} k & k' & k" \\ \ell & \ell & \ell \end{Bmatrix} \{ \sum_{ij}{}' (\underset{\sim}{u}_i^{(k)} . \underset{\sim}{u}_j^{(k)}) + (-)^{k+k'+k"} \sum_{ij}{}' (\underset{\sim}{u}_i^{(k')} . \underset{\sim}{u}_j^{(k')})$$

$$+ \sum_{ij}{}' (\underset{\sim}{u}_i^{(k")} . \underset{\sim}{u}_j^{(k")}) + \frac{N}{[\ell]} \}$$

3.3 REDUCED MATRIX ELEMENTS FOR A ONE-PARTICLE ANGULAR OPERATOR ACTING IN AN OPEN ORBITAL

From Judd[13]

$$\langle \ell^N \gamma SL \, \| U^{(k)} \| \, \ell^N \gamma' S' L' \rangle = \delta(SS') N[L,L']^{\frac{1}{2}}$$

$$\sum_{\overline{\theta}} \langle \theta \{ | \overline{\theta} \rangle \langle \theta' \{ | \overline{\theta} \rangle (-)^{\overline{L}+\ell+L+k} \begin{Bmatrix} L & k & L' \\ \ell & \overline{L} & \ell \end{Bmatrix} \tag{3.1}$$

with notation $\theta \equiv \ell^N \gamma SL$, $\theta' = \ell^N \gamma' S' L'$, $\overline{\theta} = \ell^{N-1} \, \overline{\gamma} \, \overline{S} \, \overline{L}$, γ

being any other quantum number needed to uniquely specify the state, and $\langle\theta\{|\bar{\theta}\rangle$ are coefficients of fractional parentage. In the case of N = 2 equation (3.1) simplifies to

$$\langle \ell^2 SL \,\|U^{(k)}\|\, \ell^2 S'L'\rangle = \delta(SS')2(-)^{L+k} \begin{Bmatrix} L & k & L' \\ \ell & \ell & \ell \end{Bmatrix}$$

since

$$\langle \ell^2\{|\ell\rangle = 1.$$

Racah[39] obtained a relation between the matrix elements of conjugate configurations, which on taking Judd's[32] phase, can be written as

$$\langle \ell^N \gamma SL \,\|U^{(k)}\|\, \ell^N \gamma' S'L'\rangle = (-)^{k+\frac{1}{2}(v-v'+1)}$$

$$\times \langle \ell^{4\ell+2-N} \gamma SL \,\|U^{(k)}\|\, \ell^{4\ell+2-N} \gamma' S'L'\rangle$$

$$+ \delta(\gamma\gamma')\delta(SS')\delta(LL')\delta(k0)[\ell,L]^{\frac{1}{2}}$$

where v is the seniority of state $\ell^N \gamma SL$, and v' the seniority of the state $\ell^N \gamma' S'L'$. This reduces the number of matrix elements which need to be independently calculated.

3.4 REDUCED MATRIX ELEMENTS FOR A TWO-PARTICLE ANGULAR OPERATOR ACTING IN AN OPEN SHELL

Once the one-particle reduced matrix elements have been obtained we get the two-particle reduced matrix elements from the standard result for the reduced matrix elements of a coupled product of two tensor operators[13], giving

$$\langle \ell^N \gamma SL \,\|\, (\underset{\sim}{U}^{(k)} . \underset{\sim}{U}^{(k)}) \,\|\, \ell^N \gamma' S'L'\rangle$$

$$= \delta(SS')\delta(LL') \sum_{\bar{\gamma}\,\bar{L}} \frac{(-)^{L+\bar{L}}}{[L]} \langle \ell^N \gamma L \,\|U^{(k)}\|\, \ell^N \bar{\gamma}\ \bar{L}\rangle \langle \ell^N \bar{\gamma}\ \bar{L} \,\|U^{(k)}\|\, \ell^N \gamma' L'\rangle$$

3.5 REDUCED MATRIX ELEMENTS FOR A THREE-PARTICLE ANGULAR OPERATOR ACTING IN AN OPEN ORBITAL

These are evaluated by double application of the result used in the previous case, giving

$$\langle \ell^N \gamma SL \,||\, (\underset{\sim}{U}^{(k)} . \underset{\sim}{U}^{(k')} . \underset{\sim}{U}^{(k")}) \,||\, \ell^N \bar{\gamma}\ \bar{S}\ \bar{L}\rangle$$

$$= \delta(S\bar{S})\,\delta(L\bar{L})\ \frac{(-)^{k+k'+k"}}{[L]}$$

$$\sum_{\substack{\gamma'L' \\ \gamma"L"}} \begin{Bmatrix} k & k' & k" \\ L' & L & L" \end{Bmatrix} \langle \ell^N \gamma L \,||U^{(k)}|| \ell^N \gamma"L"\rangle \langle \ell^N \gamma"L" \,||U^{(k')}|| \ell^N \gamma'L'\rangle$$

$$\langle \ell^N \gamma'L' \,||U^{(k")}|| \ell^N \bar{\gamma}\bar{L}\rangle$$

3.6 OPERATORS ACTING IN AN OPEN SHELL

Interconfigurational effective operators involve unit tensor operators $\underset{\sim}{u}^{(k)}(\ell'\ell)$ acting between orbitals of the open shell. In the case of configurations ℓ^N and $\ell'^{4\ell'+2}\ell^{N+2}$ in the ground complex we have operators

$$(\underset{\sim}{U}^{(k)}(\ell'\ell) . \underset{\sim}{U}^{(k)}(\ell'\ell))$$

$$(\underset{\sim}{U}^{(k)}(\ell'\ell) . \underset{\sim}{U}^{(k')}(\ell'\ell) . \underset{\sim}{U}^{(k")}(\ell_a\ell_a)),$$

ℓ_a is any occupied orbital of configuration $\ell'^{4\ell'+2}\ell^{N+2}$.

3.7 REDUCED MATRIX ELEMENTS FOR A ONE-PARTICLE ANGULAR OPERATOR ACTING BETWEEN ORBITALS

To evaluate reduced matrix elements of $U^{(k)}(\ell'\ell)$ we use Racah's result[39] for a one particle operator F

$$\langle \ell^N \alpha SLM_S M_L | F | \ell^{N-1} \alpha_1 S_1 L_1, \ell'; S'L'M_S'M_L'\rangle$$

$$= \sqrt{N}\ \langle \ell^N \alpha SL\{ | \ell^{N-1} \alpha_1 S_1 L_1, \ell; SL\rangle$$

$$\langle S_1 L_1, \ell_N; SLM_S M_L | f_N | S_1 L_1, \ell_N'; S'L'M_S'M_L'\rangle$$

Simplifying the matrix element

$$\langle \ell^N \alpha SL \,||U^{(k)}(\ell'\ell)||\, \ell'^{4\ell'+1}, \ell^{N+1}\alpha_2' S_2' L_2'; S'L' \rangle$$

$$= \delta(SS')\sqrt{N+1}\langle \ell^N \alpha SL \,|\}\, \ell^{N+1}\alpha_2' S_2' L_2' \rangle (-)^{2S+\ell'+L'+L_2'}$$

$$\left(\frac{[L', S_2', L_2']}{[S]}\right)^{\frac{1}{2}} \begin{Bmatrix} L & L' & K \\ \ell' & \ell & L_2' \end{Bmatrix} \sum_{\bar{S}} (-)^{2\bar{S}} [\bar{S}] \begin{Bmatrix} \frac{1}{2} & S & \bar{S} \\ \frac{1}{2} & S' & S_2' \end{Bmatrix}$$

Similarly

$$\langle \ell'^{4\ell'+1} S_1 L_1, \ell^{N+1}\alpha_2 S_2 L_2; SL \,||U^{(k)}(\ell'\ell)||\, \ell'^{4\ell'}\alpha_1' S_1' L_1', \ell^{N+2}\alpha_2' S_2' L_2', S'L'' \rangle$$

$$= \delta(SS')(-)^{k+2(S_1+S_2)-\frac{1}{2}(v+v')+S+L+\ell'} [L, L', \tfrac{1}{2}, S_1', L_1', S_2', L_2']^{\frac{1}{2}}$$

$$\sqrt{N+2}\, \langle \ell^{N+2}\alpha_2' S_2' L_2' \{| \ell^{N+1}\alpha_2 S_2 L_2, \ell \rangle$$

$$\sum_{\bar{S}\bar{L}} (-)^{\bar{S}} [\bar{S}, \bar{L}] \begin{Bmatrix} L & k & L' \\ \ell & \bar{L} & \ell' \end{Bmatrix} \begin{Bmatrix} \frac{1}{2} & S_1' & S_1 \\ S_2 & S & \bar{S} \end{Bmatrix} \begin{Bmatrix} \ell' & L_1' & L_1 \\ L_2 & L & \bar{L} \end{Bmatrix} \begin{Bmatrix} S_1' & S_2 & \bar{S} \\ \frac{1}{2} & S' & S_2' \end{Bmatrix}$$

$$\begin{Bmatrix} L_1' & L_2 & \bar{L} \\ \ell & L' & L_2' \end{Bmatrix}$$

where v is the seniority of $\ell'^{4\ell'} S_1' L_1'$, and v' the seniority of $\ell'^{4\ell'+1} S_1 L_1$.

3.8 REDUCED MATRIX ELEMENTS FOR A TWO-PARTICLE ANGULAR OPERATOR ACTING BETWEEN ORBITALS

Using the same standard method as for section (3.4)

$$\langle \ell^N SL \,||\{\underset{\sim}{U}^{(k)}(\ell'\ell) \times \underset{\sim}{U}^{(k)}(\ell'\ell)\}^0||\, \ell'^{4\ell'} S_1 L_1, \ell^{N+2} S_2 L_2; SL \rangle$$

$$= \frac{(-)^{L+k}}{[L,k]^{\frac{1}{2}}} \sum_{\bar{S}\bar{L}L'} (-)^{L'} \langle \ell^N SL \,||U^{(k)}(\ell'\ell)||\, \ell'^{4\ell'+1}, \ell^{N+1}\bar{S}\bar{L}; SL' \rangle$$

$$\langle \ell'^{4\ell'+1}, \ell^{N+1}\bar{S}\bar{L}; SL' \,||U^{(k)}(\ell'\ell)||\, \ell'^{4\ell'} S_1 L_1, \ell^{N+2} S_2 L_2; SL \rangle$$

3.9 REDUCED MATRIX ELEMENTS FOR A THREE-PARTICLE ANGULAR OPERATOR ACTING BETWEEN ORBITALS

The three-particle operator is treated by the same method of section (3.5) to give

$$\langle \ell^N SL \,||\, \{\underset{\sim}{U}^{(k)}(\ell'\ell) \times \underset{\sim}{U}^{(k')}(\ell'\ell) \times \underset{\sim}{U}^{(k'')}(\ell_a\ell_a)\}^{(0)} \,||\, \ell'^{4\ell'} S_1 L_1, \ell^{N+2} S_2 L_2; SL\rangle$$

$$= \frac{(-)^{L+k''}}{[L,k'']^{\frac{1}{2}}} \sum_{\substack{S_1'L_1', S_2'L_2' \\ S_2''L_2'', L'L''}} (-)^{L'} \begin{Bmatrix} k' & k'' & k \\ L & L'' & L' \end{Bmatrix} \langle \ell^N SL \,||\, U^{(k)}(\ell'\ell) \,||\, \ell'^{4\ell'+1}, \ell^{N+1} S_2'' L_2''; SL\rangle$$

$$\langle \ell'^{4\ell'+1}, \ell^{N+1} S_2'' L_2''; SL \,||\, U^{(k')}(\ell'\ell) \,||\, \ell'^{4\ell'} S_1' L_1', \ell^{N+2} S_2' L_2'; SL'\rangle$$

$$\langle \ell'^{4\ell'} S_1' L_1', \ell^{N+2} S_2' L_2'; SL' \,||\, U^{(k'')}(\ell_a\ell_a) \,||\, \ell'^{4\ell'} S_1 L_1, \ell^{N+2} S_2 L_2; SL\rangle$$

If $\ell_a = \ell$ or $\ell_a = \ell'$ the last reduced matrix element is one already considered. If ℓ_a is one of the core orbitals, the last reduced matrix element reduces to

$$\delta(LL')\,\delta(k''0)\; 2[\ell_a]^{\frac{1}{2}}$$

3.10 REDUCED MATRIX ELEMENTS FOR ONE-PARTICLE ANGULAR OPERATORS ACTING BETWEEN ORBITALS OF THE n = 2 SHELL

In the special case of complex $|(1^2 2^4)+\rangle$ the general results of section (3.7) simplify to

$$\langle 1s^2 2s^2\ {}^1S, 2p^2 SL \,||\, U^{(1)}(sp) \,||\, 1s^2 2s^2 S, 2p^3 S_2 L_2; SL_2\rangle$$

$$= \langle p^2 SL, p|\}p^3 S_2 L_2\rangle (-)^{L+L_2} \left(\frac{[L_2, S_2]}{[S]}\right)^{\frac{1}{2}} \sum_{\bar{S}} (-)^{2\bar{S}} [\bar{S}] \begin{Bmatrix} \frac{1}{2} & S & \bar{S} \\ \frac{1}{2} & S & S_2 \end{Bmatrix}$$

and

$$\langle 1s^2 2s^2 S, 2p^3 S_2 L; SL \,||U^{(1)}(sp)||\, 1s^2 2p^4 SL' \rangle$$

$$= (-)^{\frac{1}{2}(v+v'+1)} \left(\frac{[S_2,L]}{[S]}\right)^{\frac{1}{2}} \langle p^3\, S_2 L \{|p^2\, SL', p\rangle$$

where v is the seniority of $p^3 S_2 L$, and v' the seniority of $p^2 SL'$.

3.11 SPIN-ORBIT MATRIX ELEMENTS

For both the first and second-order spin-orbit calculations we need the matrix elements of the operator

$$\sum_i (\underset{\sim}{s}_i^{(1)} \cdot \underset{\sim}{\ell}_i^{(1)})$$

This is easiest handled by writing the operator in terms of double tensor operators $\underset{\sim}{W}^{(kk')}$. From Judd[13] we obtain

$$\langle \ell^N \alpha SLJM_J | \sum_i (\underset{\sim}{s}_i^{(1)} \cdot \underset{\sim}{\ell}_i^{(1)}) | \ell^N \alpha' S'L'J'M_J' \rangle$$

$$= \delta(JJ')\delta(M_J M_J')\ (-)^{S'+L+J} \left\{\frac{\ell(\ell+1)(2\ell+1)}{6}\right\}^{\frac{1}{2}}$$

$$\begin{Bmatrix} S & S' & 1 \\ L' & L & J \end{Bmatrix} \langle \ell^N \alpha SL \,||W^{(11)}||\, \ell^N \alpha' S'L' \rangle$$

where by definition

$$\underset{\sim}{W}^{(11)} = \sum_i \underset{\sim}{w}_i^{(11)}$$

and

$$\langle s\ell \,||w^{(kk')}||\, s'\ell' \rangle = [k,k']^{\frac{1}{2}} \delta(ss')\delta(\ell\ell')$$

Reduced matrix elements of $\underset{\sim}{W}^{(kk')}$ are given by

$$\langle \ell^N \alpha SL||W^{(kk')}||\, \ell^N \alpha' S'L' \rangle = N[S,k,S',L,k',L']^{\frac{1}{2}}$$

$$(-)^{\frac{1}{2}+\ell+S+L+k+k'} \sum_{\bar{\alpha}\bar{S}\bar{L}} \langle \ell^N \alpha SL \{|\ell^{N-1} \bar{\alpha}\bar{S}\bar{L}\rangle \langle \ell^N \alpha' S'L' \{|\ell^{N-1} \bar{\alpha}\bar{S}\bar{L}\rangle$$

$$(-)^{\bar{S}+\bar{L}} \begin{Bmatrix} S & k & S' \\ \frac{1}{2} & S' & \frac{1}{2} \end{Bmatrix} \begin{Bmatrix} L & k' & L' \\ \ell & \bar{L} & \ell \end{Bmatrix}$$

3.12 COULOMB-SPIN-ORBIT ANGULAR MATRIX ELEMENTS

For the Coulomb-spin-orbit effective operator we need the matrix elements of

$$\sum_{ij} \{ s_{\sim i}^{(1)} \times u_{\sim i}^{(t)} \times u_{\sim j}^{(k)} \}_0^{(0)}$$

which we obtain by first looking at

$$\langle \alpha J M_J | \{ U_{\sim}^{(1t)k} \times U_{\sim}^{(0k)k} \}_0^{(0)} | \alpha' J' M_J' \rangle$$

$$= \delta(JJ')\delta(M_J M_J') \frac{(-)^{J+k}}{[J]} \sum_{\alpha'' J''} \frac{(-)^{J''}}{[k]^{\frac{1}{2}}}$$

$$\langle \alpha J \| U^{(1t)k} \| \alpha'' J'' \rangle \langle \alpha'' J'' \| U^{(0k)k} \| \alpha' J \rangle$$

Expanding each of the reduced matrix elements

$$= \sum_{\alpha'' J''} (-)^J J'' \begin{Bmatrix} S & S'' & 1 \\ L & L'' & t \\ J & J'' & k \end{Bmatrix} \begin{Bmatrix} S'' & S' & 0 \\ L'' & L' & k \\ J'' & J & k \end{Bmatrix} \langle \alpha \| U^{(1t)} \| \alpha'' \rangle \langle \alpha'' \| U^{(0k)} \| \alpha' \rangle$$

and on simplifying the second 9-j symbol into a 6-j symbol we can do the sum over J" to get

$$\sum_{\alpha''} \frac{(-)^{J+L'+S'}}{[S']^{\frac{1}{2}}} \begin{Bmatrix} 1 & S & S' \\ J & L' & L \end{Bmatrix} \begin{Bmatrix} t & L & L'' \\ L'' & k & 1 \end{Bmatrix} \delta(S'S'')$$

$$\langle \alpha \| U^{(1t)} \| \alpha'' \rangle \langle \alpha'' \| U^{(0k)} \| \alpha' \rangle$$

but

$$\langle \ell^N SL \| U^{(0k)} \| \ell^N S'L' \rangle = \left(\frac{[S]}{[S]}\right)^{\frac{1}{2}} \langle \ell^N SL \| U^{(k)} \| \ell^N S'L' \rangle \delta(SS')$$

and

$$\sum_i \{ s_{\sim i}^{(1)} \times u_{\sim i}^{(t)} \}_0^{(0)} = \sum_i \{ t_{\sim i}^{(1)} \times u_{\sim i}^{(t)} \}_0^{(0)} / [s]^{\frac{1}{2}}$$

where $t_{\sim}^{(1)}$ and $u_{\sim}^{(t)}$ are unit operators acting in spin and orbital spaces respectively.

Now we have the required result

$$\langle \alpha J M_J | \sum_{ij} \{ s_i^{(1)} \times u_i^{(t)} \times u_j^{(k)} \}_0^{(0)} | \alpha' J M_J \rangle$$

$$= \sum_{\alpha''} (-)^{J+L'+S'} \begin{Bmatrix} 1 & S & S' \\ J & L' & L \end{Bmatrix} \begin{Bmatrix} t & L & L'' \\ L' & k & 1 \end{Bmatrix} \delta(S'S'') \frac{1}{[s]^{\frac{1}{2}}}$$

$$\langle \alpha \| U^{(1t)} \| \alpha'' \rangle \langle \alpha'' \| U^{(k)} \| \alpha' \rangle$$

with

$$\underset{\sim}{U}^{(1t)} = \frac{\underset{\sim}{W}^{(1t)}}{[1,t]^{\frac{1}{2}}}$$

agreeing with the result of Rajnak and Wybourne[2].

The operator appearing in the off-diagonal effective operator for the Coulomb-spin-orbit interaction is

$$\sum_{ij} \{ s_i^{(1)} \times u_i^{(t)}(\ell'\ell) \times u_j^{(k)}(\ell'\ell) \}_0^{(0)}$$

$$= (3/2)^{\frac{1}{2}} \{ \underset{\sim}{U}^{(1t)}(\ell'\ell) \times \underset{\sim}{U}^{(0k)}(\ell'\ell) \}_0^{(0)}$$

the matrix elements of which are obtained as in the previous case.

CHAPTER 4

EVALUATION OF THE RADIAL INTEGRALS

4.1 INTRODUCTION

Radial functions, determined by the central field, are needed in evaluating radial integrals which weight the angular operators in the effective operators. Taking the central field to be hydrogenic we shall be able to analytically evaluate integrals involving discrete states, but not for continuum states. Equalities are found between discrete state Coulomb integrals, for which no general proof has been found.

4.2 THE GENERAL COULOMB RADIAL INTEGRAL

The Coulomb radial integral was defined in chapter 1 as

$$R^k(ab,cd) = \int_0^\infty \int_0^\infty \frac{r_<^k}{r_>^{k+1}} R_a(r_1)R_b(r_2)R_c(r_1)R_d(r_2)r_1^2 r_2^2 dr_1 dr_2$$

where $r_<$ and $r_>$ are the lesser and greater of r_1 and r_2 respectively. This integral can be written without the $r_<$ and $r_>$ as

$$R^k(ab,cd) = \int_0^\infty R_a(r_1)R_c(r_1)r_1^{-k+1} \int_0^{r_1} R_b(r_2)R_d(r_2)r_2^{k+2} dr_2 dr_1$$

$$+ \int_0^\infty R_b(r_2)R_d(r_2)r_2^{-k+1} \int_0^{r_2} R_a(r_1)R_c(r_1)r_1^{k+2} dr_1 dr_2 \quad (4.1)$$

being more amenable to analytic evaluation. We are using the notation that letters a, b, c and d stand for the set of quantum numbers needed to specify the radial wavefunction for the first, second, third and fourth electrons in symbol $R^k(ab,cd)$.

4.3 COULOMB RADIAL INTEGRALS FOR DISCRETE HYDROGENIC FUNCTIONS

In the hydrogenic approximation the radial functions are the conventional hydrogenic radial wavefunctions for nuclear charge Z[6,11,14,40]. The complete set of such functions contains two infinite sets, one set being countable and associated with the discrete spectrum, and the other being uncountable and associated with the continuum spectra of the hydrogen atom.

The hydrogenic radial functions are expressed in terms of the confluent hypergeometric function defined by[41]

$$F(\alpha,\rho;z) = \frac{\Gamma(\rho)}{\Gamma(\alpha)\Gamma(\rho-\alpha)} \int_0^1 e^{zt}\, t^{\alpha-1}(1-t)^{\rho-\alpha-1}\, dt \qquad (4.2)$$

for $R(\alpha) > 0$, $R(\rho-\alpha) > 0$ and $t^{\alpha-1}$, $(1-t)^{\rho-\alpha-1}$ taking their principal values. For the discrete functions

$$\alpha = -n+\ell+1, \quad \rho = 2\ell+2, \quad z = \frac{2Zr}{n}$$

and then the confluent hypergeometric function is expressible as a terminating power series of z giving

$$R_{n\ell}(r) = Z^{-3/2} \frac{n}{n^2} \{(n-\ell-1)!(n+\ell)!\}^{\frac{1}{2}} \left(\frac{2Zr}{n}\right)^{\ell} e^{-\frac{Zr}{n}} \sum_{s=0}^{n-\ell-1} \frac{\left(-\frac{2Zr}{n}\right)^s}{(n-\ell-1-s)!(2\ell+1+s)!s!} \qquad (4.3)$$

With these radial functions the Coulomb integral (4.1) involves evaluation of integrals of the form

$$\int_0^\infty e^{-\alpha r_1} r_1^p \int_0^{r_1} e^{-\beta r_2} r_2^q \, dr_2 dr_1$$

$$= \frac{p!q!}{\alpha^{p+1}\beta^{q+1}} - \sum_{s=o}^{q} \frac{q!}{(q-s)!} \frac{(p+q-s)!}{(\alpha+\beta)^{p+q+1-s}\beta^{s+1}}$$

On using the identity

$$1 - x^{b+1} \sum_{r=0}^{a} \frac{(b+r)!}{r!b!} (1-x)^r = (1-x)^{a+1} \sum_{r=0}^{b} \frac{(a+r)!}{r!a!} x^r$$

the radial integral becomes

$$R^k(ab,cd) = Z\, A(ab,cd) \sum_{S_1=0}^{n_a-\ell_a-1} \cdots \sum_{S_4=0}^{n_d-\ell_d-1} A(S_1)B(S_2)C(S_3)D(S_4) \times I(S_1S_2, S_3S_4)$$

where

$$A(ab,cd) = \frac{2^4}{(n_a n_b n_c n_d)^2} \{(n_a-\ell_a-1)!(n_a+\ell_a)!\ldots(n_d-\ell_d-1)!(n_d+\ell_d)!\}^{\frac{1}{2}} \times \left(\frac{2}{n_a}\right)^{\ell_a} \cdots \left(\frac{2}{n_d}\right)^{\ell_d}$$

$$A(S_1) = \frac{\left(-\frac{2}{n_a}\right)^{S_1}}{(n_a-\ell_a-1-S_1)!(2\ell_a+1+S_1)!S_1!}$$

with similar expressions for $B(S_2)$, $C(S_3)$ and $D(S_4)$.

$$I(S_1S_2, S_3S_4) = \frac{q!}{\alpha^{q+1}(\alpha+\beta)^{p+1}} \sum_{r=0}^{q} \frac{(p+r)!}{r!} \left(\frac{\alpha}{\alpha+\beta}\right)^r + \frac{y!}{\beta^{y+1}(\alpha+\beta)^{x+1}} \sum_{r=0}^{y} \frac{(x+r)!}{r!} \left(\frac{\beta}{\alpha+\beta}\right)^r$$

where

$$p = \ell_b + \ell_d + 2 + k + S_2 + S_4$$

$$q = \ell_a + \ell_c + 1 - k + S_1 + S_3$$

$$x = \ell_a + \ell_c + 2 + k + S_1 + S_3$$

$$y = \ell_b + \ell_d + 1 - k + S_2 + S_4$$

$$\alpha = (n_a + n_c)/n_a n_c$$

$$\beta = (n_b + n_d)/n_b n_d$$

We see that the Coulomb radial integral, for discrete functions, is proportional to Z. If Coulomb integrals

involving continuum functions have the same Z dependence, Layzer's Z-expansion for the non-relativistic energy of an atom follows from perturbation theory.

The result above was programmed using powers-of-prime-numbers routines to do the arithmetic. A table of all Coulomb radial integrals for $n \leqslant 4$ and allowed ℓ with the parity-allowed k values is contained in Appendix E. It is interesting to note that very large primes appear for small values of n, ℓ, and k suggesting that a group theoretical treatment of these integrals would be difficult.

4.4 EQUALITIES BETWEEN COULOMB RADIAL INTEGRALS FOR DISCRETE HYDROGENIC FUNCTIONS

Having used power-of-prime-number arithmetic in evaluating the table of discrete Coulomb integrals no round-off errors are present making any equalities or proportionalities found exact.

The following equalities were found

R0(2s2s,2s1s) = R0(2p2s,2p1s)

R0(3p3p,3p2p) = R0(3d3p,3d2p)

R0(4d4d,4d3d) = R0(4f4d,4f3d)

R1(2p2p,2s2s) = R2(2p2p,2p2p)

R2(4f2p,4p2p) = -R1(4f2p,4d2s)

R0(4d4d,4d4d) = R0(4f4p,4f4p)

R3(5g5g,5p5p) = R6(5g5g,5d5d)

The first three satisfy the relation

R0(nn-2 nn-2,nn-2 n-1 n-2) = R0(nn-1 nn-2,nn-1 n-1 n-2)

which has been verified by calculation up to n = 9. On looking at the complexity of these integrals the equalities are quite astounding. Cunningham[42] has shown that hydrogenic radial functions form an irreducible representation of the non-compact group O(2,1) which could lead to a group theoretical explanation of these equalities. We need to be able to write the Coulomb interaction in terms of O(2,1) tensor operators. Cunningham has successfully done this for the operator r^k but the Coulomb radial part $r_<^k/r_>^{k+1}$ is much more elusive, and presents an interesting problem in group theory.

4.5 COULOMB RADIAL INTEGRALS FOR CONTINUUM HYDROGENIC FUNCTIONS

Continuum hydrogenic radial functions are expressed in terms of the confluent hypergeometric function (4.2) with

$$\alpha = \frac{i}{k} + \ell + 1, \quad \rho = 2\ell + 2, \quad z = 2ikZr$$

k any non-negative real number. Since the confluent hypergeometric function is now defined by an integral over the complex variable z, and α is also complex, it is not expressible as a terminating power series.

The function $F(\alpha,\rho;z)$ has the same dependence on nuclear charge Z in both continuum and discrete cases, so it seems reasonable to assume the same Z-dependence for integrals involving continuum functions as is found for the discrete functions alone.

Safronova *et al.*[43] have managed to obtain Coulomb integrals involving simple discrete and continuum functions by using special forms of the integral representation of the

confluent hypergeometric function of a complex variable. No general result has been obtained because of the complexity of the general contour integral.

4.6 THE GENERAL SPIN-ORBIT RADIAL INTEGRAL

The general spin-orbit radial integral is defined as

$$\zeta_{n\ell,n'\ell} = \frac{1}{2c^2} \int_0^\infty R_{n\ell}(r)\ R_{n'\ell}(r)\ \frac{1}{r}\frac{\partial U}{\partial r}\ r^2 dr$$

where U is the symmetric electrostatic field the electron moves in.

4.7 THE SPIN-ORBIT RADIAL INTEGRAL FOR HYDROGENIC FUNCTIONS

The spin-orbit radial integral in the hydrogenic approximation is

$$\zeta_{n\ell,n'\ell} = \int_0^\infty r^{-3}\ R_{n\ell}(r)\ R_{n'\ell}(r)\ r^2 dr$$

On substituting the series expansion for discrete hydrogenic functions we see that we must evaluate the definite integral

$$\int_0^\infty e^{-\alpha r} r^p dr = \frac{p!}{\alpha^{p+1}} \qquad \text{for } p > 0$$

This integral is divergent for p less than zero, which happens only if ℓ is an s-orbital. Since operator $(\underset{\sim}{s}_i^{(1)} \cdot \underset{\sim}{\ell}_i^{(1)})$ vanishes when it acts on an s-orbital we obtain an indeterminant form. Divergence of the radial integral is found to be a consequence of the non-relativistic assumption that the difference between the total energy of the electron and the central field is much less than the rest mass of the electron. This is not the case for small distances from the

nucleus where the electrons probability of being found is greatest for an s-orbital. On using the relativistic form of the hydrogen Hamiltonian it can be shown that the above integral is convergent, resulting in zero contribution from s-orbitals[6].

The spin-orbit radial integral is given by

$$\zeta_{n\ell,n'\ell} = Z^3 \frac{2^2}{(n\ n')^2} \{(n-\ell-1)!(n+\ell)!(n'-\ell-1)!(n'+\ell)!\}^{\frac{1}{2}} \left(\frac{2}{n}\right)^{\ell} \left(\frac{2}{n'}\right)^{\ell}$$

$$\sum_{s=0}^{n-\ell-1} \sum_{s'=0}^{n'-\ell-1} \frac{\left(-\frac{2}{n}\right)^{s} \left(-\frac{2}{n'}\right)^{s'} (2\ell+s+s'-1)!}{(n-\ell-1-s)!(n'-\ell-1-s')!(2\ell+1+s)!(2\ell+1+s')!s!s'!} \times \frac{1}{\alpha^{2\ell+s+s'}}$$

where

$$\alpha = (n+n')/nn'$$

We see that the total spin-orbit matrix element depends on the fourth power of Z.

If spin-orbit radial integral $\zeta_{n\ell,n'\ell}$ used in the effective operators listed in Appendix A are the integrals of this section divided by the positive square root of the appropriate energy difference. This is to include the energy denominator required by perturbation theory.

CHAPTER 5

CALCULATIONS FOR THE CI ISOELECTRONIC SEQUENCE

5.1 INTRODUCTION

The carbon atom has six electrons so the ground complex will be $|(1^2 2^4), p\rangle$. Both parities are allowed, but it is known from experiment[44] that the positive parity complex is energetically lowest, hence we shall only consider this case.

The configurations contained in $|(1^2 2^4), +\rangle$ are

$$1s^2 2s^2 2p^2$$

$$1s^2 2p^4$$

both with terms ^1SD and ^3P.

Since the Coulomb operator is diagonal in both S and L the energy matrix separates into three independent blocks, one for each term, each diagonalized separately.

The example of CI was chosen because it is difficult enough to involve more than one configuration in the ground complex, but with an open p-orbital the number of matrix elements needed in evaluating second-order effective operators is small enough not to cause any computing problems from the lack of computer core storage. His example will allow advantages of the effective operator formalism to be apparent, and will lead to suggestions for the improvement of previous calculations.

5.2 FIRST-ORDER COULOMB CORRECTIONS

For the first-order corrections we require the matrix elements of the Coulomb operator in the ground complex. These are readily obtained by standard methods[6,11,13] and have been

given by Layzer[5] for configurations $1s^2 2s^q 2p^r$, q and r taking all allowed values.

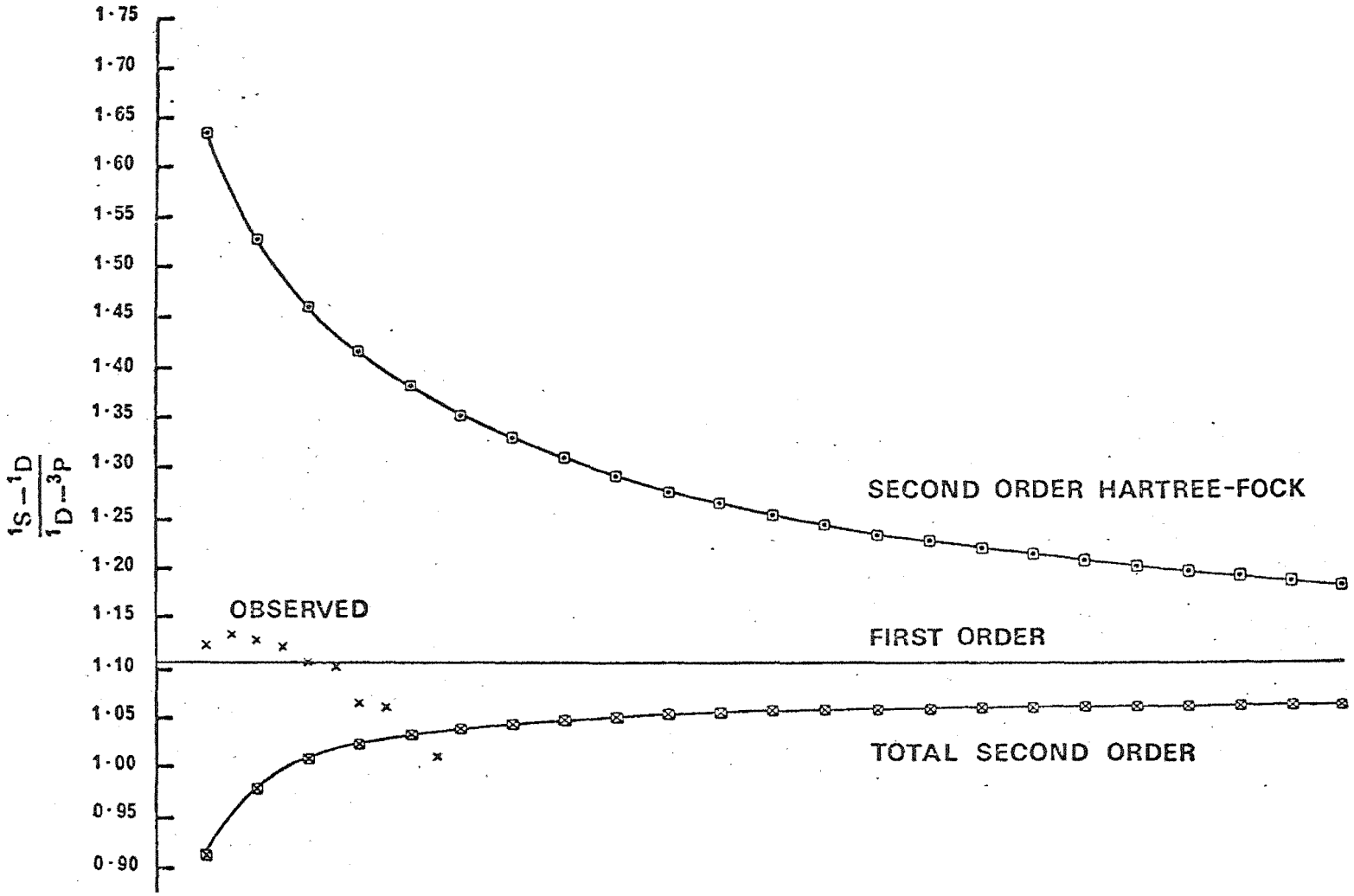
To zero-order all terms of the complex are degenerate, but the first-order Coulomb correction removes this leaving only the level degeneracy of each term. A measure of the term structure, independent of absolute energies, is the energy difference ratio

$$\frac{^1S - {}^1D}{^1D - {}^3P}$$

with the notation that ^1S stands for the energy of the ^1S term etc.

This particular ratio is chosen since to first-order in the p^2 configuration it is independent of the central field used[6,11] and has the value 3/2, whereas the observed value for CI is 1.12[44], suggesting that this ratio may be a good measure of the success in mixing in of excited configurations for perturbative corrections. Being a ratio of differences of term energies it will be very sensitive to the movement of one term with respect to the others, but will not show any magnification present in the calculated term structure. This ratio has been used to determine which configurations to use in a multiconfigurational Hartree-Fock calculation so as to obtain a 'constant error' in the energy eigenvalues[45]. A flaw with such a method is that by judiciously choosing the configurations the calculated value of the energy difference ratio can be made to correspond to the observed value but magnification of term structure is ignored, as shown in our first-order result.

On diagonalizing the sum of zero and first-order energy matrices in the complex, we find the absolute energies are


1·75
1·70
1·65
1·60
1·55
1·50
1·45
1·40
1·35
1·30
1·25
1·20
1·15
1·10
1·05
1·00
0·95
0·90
$\frac{^1S - {}^1D}{^1D - {}^3P}$
SECOND ORDER HARTREE-FOCK
OBSERVED
FIRST ORDER
TOTAL SECOND ORDER

much too high, and the energy difference ratio, which is independent of the nuclear charge, becomes 1.08. The observed value of this ratio varies slightly along the isoelectronic sequence as shown in figure 1. Even though the first-order value for the energy difference ratio is close to that observed, magnification in the calculated term structure is about two, viz. term separations $^1S - {}^1D$ and $^1D - {}^3P$ are about twice that observed.

5.2 SECOND-ORDER COULOMB CORRECTIONS FROM DISCRETE ORBITALS

An intermediate configuration involves excitation of at least one electron into an orbital $n\ell$ lying energetically above its ground orbital. The effective operators dependence on principal quantum numbers is in the radial integrals and energy denominator, not in the angular matrix elements, so the sum over n may be carried out first. This will give an effective radial integral divided by an effective energy difference which when used in the effective operator, in place of the radial integral divided by the energy difference, gives the accumulated correction for all the orbitals included in the sum over n. Alternatively the effective operator may be calculated for each case, obtaining the correction introduced by each configuration. The second method allows us to see which excitations are the important ones, so we have done the partial sum over discrete states this way.

Corrections to the ground state energies of each term of CI, and the energy difference ratio, for first and the major second-order terms are listed in Appendix B. Energy units are cm^{-1}. The zero-order ground state energy is listed followed by the first-order energy corrections to each term of

configurations $1s^2 2s^2 2p^2$ and $1s^2 2p^4$. After the ^1D term corrections follows the energy difference ratios in the same order. Next come second-order corrections arranged in the same manner. The energy corrections shown are differences between the diagonalized energy matrices after addition of the appropriate effective operator matrix elements and the diagonalized energy matrix before this addition. The diagonalized energies depend on corrections already considered making the listed corrections dependent on the order in which configurations are considered. On reordering the configurations it was found that the energy corrections charged by a few percent, indicating that trends apparent in the given sequence of configurations are not dependent on the order of treatment. A similar result holds for the energy difference ratio.

Total energies for each term of both configurations present in complex $|(1^2 2^4),+\rangle$ are given at the very end of Appendix B.

Major second-order corrections to the ground state energy are seen to come from single-particle excitation 1s → ns, 2s → ns and 2p → np. Corrections from excitations 2s → 3s are almost twenty times that of 1s → 3s, while 2p → 3p corrections are only a little larger than for 2s → 3s.

The major term in the effective operator for 1s → ns species of excitations is the one involving the direct radial integral where the passive and excited electrons come from the same orbital. Radial integral RO(3s1s,1s1s) is twice that of RO(3s2s,2s2s) but the energy differences are 8/9 and 5/36 respectively making the square of the radial integral divided by the energy difference largest for the 2s excitation

accounting for the observed difference. Similarly for the 2p → 3p excitation involving direct integrals of rank zero and two for passive 2p electrons. As the excited orbitals principal quantum number increases the Coulomb integrals quickly decrease and energy denominators increase making the corrections rapidly fall. By n = 5 the 2p → np excitation contributes only one hundredth that of n = 3. Rapid convergence is found in all cases.

The major two-particle excitation is $2s^2 \rightarrow 2p3p$ which also produces a very large correction in the energy of configuration $1s^2 2p^4$. This is the two-particle contribution with the smallest energy denominator, and also the 2s and 2p orbitals major maxima almost overlap. No other multiple-excitation produces corrections over two thousand wavenumbers, and very few give more than a few hundred wavenumbers.

Effective operators, diagonal in the configuration, represent the sum of squares of matrix elements all divided by a negative energy difference and must therefore be negative. Corrections to each term can be ensured to be negative only if the Coulomb operator can not couple the different configurations of the ground complex through an intermediate configuration. A number of two-electron excitations listed give exactly zero contributions, indicated by 0.0. These arise from the diagonality of the Coulomb operator in the total spin and angular momentum quantum numbers. For example, intermediate configuration $2s^2 2p^2 3s4d$ gives zero contribution as it requires the matrix element

$$\langle 3s4d S_1 L_1 | (\underset{\sim}{C}_1^{(k)} . \underset{\sim}{C}_2^{(k)} | 1s^2\ {}^1S \rangle$$

and S_1L_1 can only be ^1D or ^3D. Corrections smaller than -0.05 cm^{-1} are shown as -0.0.

It was shown in chapter 1 that we have the non-relativistic energy expansion

$$E = E_0Z^2 + E_1Z + E_2 + \ldots$$

where E_0 is the zero-order energy, E_1 the first-order and E_2 the second-order perturbative energies. With the ground complex containing two configurations E_1 and E_2 are 2 x 2 matrices, given an energy matrix E which must be diagonalized for each Z to obtain term energies. We shall use the notation E0, E1 and E2 to refer to the diagonalized energies up to zero, first and second-order respectively. The symbols E_0,E_1, E_2,... refer to a particular order of perturbation, while E0, E1, E2 ... refer to the diagonalized energies up to and including that particular order. If only Hartree-Fock excitations are included in E_2 we write E_2(H.F) and the diagonalized energy is referred to as E2(H.F) . Values of E0, E1, E2, E2(H.F) , in cm^{-1}, and the energy ratios for approximations E2 and E2(H.F) are tabulated in Appendix C for nuclear charge Z from six to fifty. Only the ground configuration $1s^22s^22p^2$ is considered. Second-order energy matrix E2 contains the contributions from all intermediate configurations listed in Appendix B, and E2(H.F) all the Hartree-Fock excitations contained in E2. The energy matrices (in cm^{-1}) are

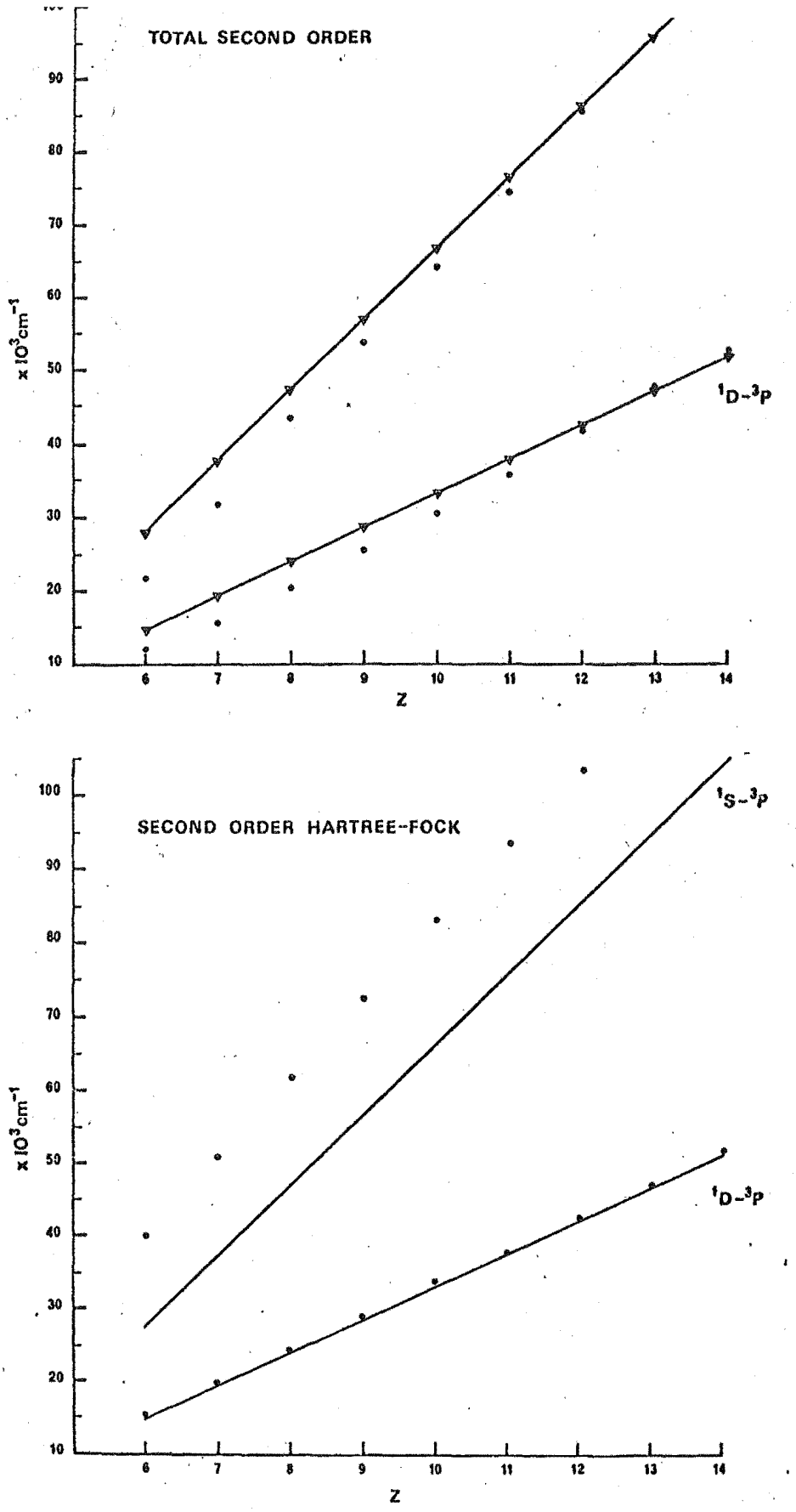


Figure 2: Term energy differences for the CI isoelectronic sequence.

	^1S	^3P	^1D
E_1	727,491	715,917	720,547
	12,860	-6,430	-6,430
	787,683	776,109	780,739
E_2	-589,380	-563,254	-575,984
	4,808	-1,284	-2,798
	-638,667	-603,493	-620,119
E_2(H.F)	-582,121	-551,032	-562,698
	- 28,288	- 25,179	- 31,027
	- 25,394	- 24,198	- 24,129

Calculated energy difference ratios for nuclear charge Z from six to fifty are graphed in figure 1 along with the observed values for Z from six to fifteen. 'Total second-order' on the graph refers to E2.

The second-order Hartree-Fock energy difference ratio is much too large for Z of six, while second-order is too low, but closer than the Hartree-Fock value. Both ratios approach the first-order value monotonically as the nuclear charge increases. Note that the first-order value gives about the mean observed value. As Z increases the E_2 and E_2(H.F) terms in the energy expansion become less important causing both second-order and Hartree-Fock energy ratios to asymptotically approach the first-order value of 1.108.

In figure 2 energy differences $^1S - ^3P$ and $^1D - ^3P$ are plotted for both E2 and E2(H.F). Observed points[44], shown in the top graph only, are joined by the solid line shown in both graphs. The dots are the calculated points. We see that the

the E2 values are better overall, but the E2(H.F) are very good for $^1D - {}^3P$ and poor for $^1S - {}^3P$. Excitation series causing large changes in the energy difference ratio are $2s \rightarrow ns$, $2p \rightarrow np$ and $2s^2 \rightarrow 2pnp$. The last case, which is a non-Hartree-Fock contribution, producing the largest change from 1.62 down to 0.97, is the main cause of the difference between Hartree-Fock and second-order calculations involving discrete orbitals.

Linderberg[46] has calculated the contribution to E_2 from single-particle excitations by means of a variational method which gives an upper bound for such corrections. Using the value so obtained the energy difference ratio is 0.508 and the ground state energy is about 10^5 cm^{-1} lower than ours. Our second-order correction, containing only discrete orbitals, contains approximately eighty-five percent of Linderberg's value. The continuum probably contributes the remaining fifteen percent, as two-particle corrections do not appreciably alter the absolute energies. The calculated energy difference $^1S - {}^1D$ is 1.04 times that observed showing that even though our second-order energy difference ratio is not as good as the first-order value there is very little magnification of the term structure to second order.

5.4 SECOND-ORDER COULOMB CORRECTIONS FROM CONTINUUM ORBITALS

Schull and Löwdin[47] have quite convincingly shown that the continuum functions are important in our perturbative calculations. They have shown that the reason discrete radial functions

$$L_n^l \left(\frac{2Zr}{n}\right) e^{-\frac{Zr}{n}}$$

used by Taylor and Parr[50] in a configurational mixing calculation gave a poor convergence compared with the complete set

$$L_n^1 (2Zr)\ e^{-Zr}$$

taken by Hylleraas[51], is associated with the incompleteness of Taylor and Parr's functions. Safronova *et al.*[43] have verified the importance of continuum states in their calculation for the Hartree-Fock excitations of a 1s electron in the helium problem. They found that the continuum contributes about the same as the discrete states to E_2(H.F).

Very little has been written about atomic continuum spectra and the associated eigenfunctions[14,40]. The hydrogenic radial continuum functions are expressed as contour integrals, which makes them difficult to work with and has probably been the main reason for their neglect. Kelly[48] has used an asymptotic form of the radial functions which he normalizes in a large spherical box, the size of which is taken to be of the order of 100 au. This asymptotic approximation seems to be often made[49].

Since few texts deal with continuum functions we shall look at the normalization applicable for series expansions[14] as given by perturbation theory.

A square integrable function $\phi(\underset{\sim}{r})$ is expressible as a Fourier series over any complete set of functions $\psi(\underset{\sim}{r},\theta)$, θ being some variable which can be used as a label to distinguish between the functions of the complete set. If θ takes discrete values θ_n only, then

$$\phi(\underset{\sim}{r}) = \sum_n a_n \psi(\underset{\sim}{r},\theta_n)$$

or if θ is a continuous variable

$$\phi(\underset{\sim}{r}) = \int a(\theta)\ \psi(\underset{\sim}{r},\theta)\ d\theta,$$

the integral being taken over the principal range of θ. The most general case is for θ to have both discrete and continuous ranges, such as for the energy in the hydrogen problem. Now

$$\phi(\underset{\sim}{r}) = \sum_n a_n\ \psi(\underset{\sim}{r},\underset{\sim}{\theta}_n) + \int a(\theta)\ \psi(\underset{\sim}{r},\theta)d\theta \tag{5.1}$$

Since $\phi(\underset{\sim}{r})$ is assumed square integrable, without loss of generality assume that

$$\int \phi^*(\underset{\sim}{r})\ \phi(\underset{\sim}{r})d\underset{\sim}{r} = 1 \tag{5.2}$$

which implies

$$\sum_n a_n^*\ a_n + \int a^*(\theta)\ a(\theta)\ d\theta = 1$$

and by substituting (5.1) into (5.2) we see that

$$a_n = \int \phi(\underset{\sim}{r})\ \psi^*(\underset{\sim}{r},\theta_n)\ d\underset{\sim}{r} \tag{5.3}$$

$$a(\theta) = \int \phi(\underset{\sim}{r})\ \psi^*(\underset{\sim}{r},\theta)\ d\underset{\sim}{r} \tag{5.4}$$

Expansion (5.1) for function $\phi(\underset{\sim}{r})$, leading to the coefficients given by equations (5.3) and (5.4), assumes a definite normalization for the basis states $\psi(\underset{\sim}{r},\theta)$. Substituting equation (5.4) back into (5.1) gives

$$a(\theta) = \int a(\theta')\left(\int \psi(\underset{\sim}{r},\theta')\psi(\underset{\sim}{r},\theta)d\underset{\sim}{r}\right) d\theta'$$

which is true for all θ. Hence we must have

$$\int \psi(\underset{\sim}{r},\theta')\ \psi(\underset{\sim}{r},\theta)\ d\underset{\sim}{r} = \delta(\theta,\theta') \tag{5.5}$$

where $\delta(\theta,\theta')$ is Dirac's delta function. If one does not like

the idea of equating two infinities (5.5) may be written as

$$\int\int \psi(\underset{\sim}{r},\theta)\ \psi^*(\underset{\sim}{r},\theta)\ d\underset{\sim}{r}d\theta = 1 \qquad (5.6)$$

Bethe and Salpeter[40] have normalized the hydrogenic continuum functions in this way, taking θ to be the energy.

Safronova *et al.*[43] have evaluated various Coulomb integrals involving continuum functions by using special forms of the confluent hypergeometric function. Unfortunately the general result has not been obtained since the confluent hypergeometric function cannot be written in a form amenable to carrying out the required integrals and we are forced to look at numerical methods.

For continuum functions the integrand of the integral representation of the confluent hypergeometric function, see section 4.5, is an oscillating function of $2kZr$, which in turn makes the radial function oscillatory. The rate of oscillation increases with energy as k^2. With rapidly varying integrands multiple numerical integration cannot be expected to give accurate estimates of the required integrals, but programmes were written and tested on discrete function integrals. On terminating the discrete functions when their argument was less than 10^{-3} gave Coulomb integrals accurate to three significant figures. A correction of about -3.3×10^6 cm^{-1} was obtained for each term in the ground configuration for excitations $2p \rightarrow kp$, k taking the range 0 to 1.5. This result is much bigger than expected, and it is doubtful if any conclusion can be drawn from it because of the inaccuracies of the method.

5.5 FIRST-ORDER SPIN-ORBIT CORRECTIONS

The Coulomb interaction leaves the levels of a given term degenerate. This degeneracy is lifted by the spin-orbit operator.

Taking the perturbation as the sum of the Coulomb and spin-orbit operators we note that it no longer commutes with S and L, but with the total angular momentum J. Consequently the perturbation matrix elements are not diagonal in SL as before, and are only diagonal in J. This results in the energy matrix breaking up into blocks according to J, and not SL as for the Coulomb operator alone. If we diagonalize the energy matrix containing zero, first- and second-order discrete Coulomb corrections discussed in the previous sections, along with the first-order spin-orbit correction as given in Appendix D is obtained. This gives a separation between the levels of the ^3P term ten times larger than observed ($^3P_0$-$^3P_1$ = 16.4 cm^{-1}, $^3P_0$-$^3P_2$ = 43.5 cm^{-1})[44]. This is not unexpected since we are assuming that the 1s and 2s electrons do not screen the 2p electrons from the nucleus so they see the entire nuclear charge of 6 a.u. With the spin-orbit interaction being proportional to Z^4 a small amount of screening would substantially affect the fine structure. Hydrogen fine structure calculated as the first-order spin-orbit correction is in good agreement with experiment supporting the concept of screening.

5.6 SECOND-ORDER SPIN-ORBIT CORRECTIONS

As explained in chapter 2 the second-order spin-orbit correction involves both spin-orbit-spin-orbit and Coulomb-spin-orbit parts. The first of these depends on Z^6, the second on Z^3. Calculation shows that the spin-orbit-spin-orbit part

is a factor of a thousand down on the Coulomb-spin-orbit part for CI.

The entire second-order spin-orbit correction for each configuration considered is given in Appendix D. It is seen that there is good convergence but the fine structure is still too large.

Excitations involved at second-order promote a p-electron since the spin-orbit operator cannot interact with s-electrons. Hence the p-electrons are still screened from the nucleus. We expect the first effects of screening to show in third-order. The sequence of excitations

$$1s^2 2s^2 2p^2 \xrightarrow{\text{Coulomb}} 1s^2 2s 2p^2 3s \xrightarrow{\text{Coulomb}} 1s^2 2s^2 2p 3p$$

$$\xrightarrow{\text{Spin-orbit}} 1s^2 2s^2 2p^2$$

has been estimated to reduce the separation between levels $^3P_0$ and $^3P_1$ by about 15 cm^{-1} making it appear that third-order terms must be included before we can expect reasonable fine structure results.

5.7 HIGHER-ORDER SPIN-ORBIT CORRECTIONS

With the relativistic corrections alone giving an energy expansion in increasing powers of Z we have no prior knowledge of how good a given approximation will be as the neglected terms are proportional to even higher powers of Z and therefore increase with importance as Z increases along an isoelectronic sequence. The second-order calculations indicate that the $(\text{spin-orbit})^n$ interactions, in the n^{th}-order correction, are much smaller than the $\text{Coulomb-(spin-orbit)}^{n-1}$ interactions, at the beginning of an isoelectronic sequence,

so we expect that to third order the important fine structure corrections will come from the Coulomb-Coulomb-spin-orbit part which is independent of Z. Permutations of the three operators in an n^{th}-order interaction, $\text{Coulomb}^{m}\text{-(spin-orbit)}^{n-m}$, is naturally also an allowed interaction, and all such interactions have the same Z dependence.

CHAPTER 6

CONCLUSION

6.1 Z-EXPANSION AS A STATEMENT OF PERTURBATION THEORY

We have shown that the Z-expansion

$$E = E_0 Z^2 + E_1 Z + E_2 + \ldots$$

for the non-relativistic energy of an atom or ion is nothing more than a perturbation expansion in which the entire Coulomb repulsion is treated as a perturbation on the hydrogen-like Hamiltonian

$$H_0 = \sum_i \left(\frac{P_i^2}{2} - \frac{Z}{R_I}\right)$$

The first two terms in this expansion involve states of a single complex and can therefore be obtained to any degree of accuracy required. The only thing preventing an exact solution to first order is the diagonalization of the energy matrix, required if more than one configuration is present in the complex.

The third term E_2, given by second-order perturbation theory, involves a summation over all the states of the zero-order Hamiltonian other than the ones being perturbed. For the hydrogen-like Hamiltonian H_0 this sum is over two infinite sets of functions, describing the discrete and continuum states, which together form a complete set. Neither of these infinite sums has been evaluated, but partial summations have been carried out by various methods. The sum over discrete orbitals has been partially evaluated for helium by Scherr[52]

and by Layzer *et al.*[4] using conventional methods of evaluating each matrix element separately. Linderberg[53] has obtained the entire Hartree-Fock part of E_2 for various configurations involving s-orbitals. Further references to the method used in Linderberg's calculation will be found in Sharma and Wilson's[54] work. Some of the non-Hartree-Fock parts of E_2 for helium have been obtained by Sharma and Bowtell[55]. The entire E_2 term for lithium has been obtained by Chisholm and Dalgarno[56]. The method used for evaluating these contributions, without explicitly carrying out the summations, involves the solutions of a set of uncoupled differential equations which has been done only for s-orbitals. Linderberg[46,57] has used the variational method to estimate the Hartree-Fock and total value of E_2 for a number of ground configurations. Safronova *et al.*[43] have managed to obtain analytic forms for the Coulomb radial integrals required for simple configurations and by using their asymptotic forms effectively summed over all the discrete and continuum states. We have shown that by the use of Rajnak and Wybourne's equivalent operators[1-3], the sum over all intermediate quantum numbers of states belonging to some configuration coupled up to a total SL can be obtained in terms of radial integrals involving excited orbitals and angular matrix elements within the ground complex. As we have a series representation for the discrete radial functions[6,11,14,4] the Coulomb integrals over discrete states have been evaluated making it possible to obtain each of the partial sums over intermediate quantum numbers without invoking numerical methods.

No way of evaluating continuum Coulomb radial integrals analytically has been found yet. Numerical methods were tried without success. Refinement of the numerical methods may improve this estimate, but it is felt that further work on the analytic methods is preferable.

6.2 MAJOR SECOND-ORDER CORRECTIONS

Using effective operators to obtain discrete contributions to E_2 for the CI isoelectronic sequence we have been able to see which configurations contribute to the absolute energies of each term, and which alter the term structure.

We found that the major correction to the ground state absolute energy comes from single-particle excitation, and that these corrections quickly converge. Two-particle excitation $2s^2 \rightarrow 2pnp$ has a large effect on the term structure as reflected in the energy difference ratio but does not contribute greatly to the ground state's absolute energy.

Continuum contributions are estimated to be fifteen percent of E_2, which we arrived at by comparing Linderberg's[46] variational value with our result, noting that the two-particle excitations contribute little to the absolute energies.

Important one-particle excitations are all included in the Hartree-Fock energy. This suggests that these corrections should be considered by a more appropriate method, such as that used by Linderberg[53], and Sharma and Wilson[54], and introduce the second-order radial correlation (i.e. non-Hartree-Fock) by our method.

6.3 CHOICE OF ZERO-ORDER HAMILTONIAN

It may be possible to overcome the difficulties of the continuum by taking a zero-order Hamiltonian which only has a discrete spectrum. Such an example is the harmonic oscillator Hamiltonian[58]

$$H_{HO} = \tfrac{1}{2} \sum_i (\underset{\sim}{p}_i^2 - \underset{\sim}{r}_i^2)$$

Following Tolmachev[59] transform the variables of the eigenvalue problem

$$H_{NR}(\underset{\sim}{r})\ \Psi(\underset{\sim}{r}) = E\ \Psi(\underset{\sim}{r})$$

as

$$\underset{\sim}{r} = Z\ \underset{\sim}{\rho}$$

and define

$$\Psi(r) = \Phi(\frac{\underset{\sim}{r}}{Z}), \qquad \varepsilon = \frac{E}{Z^2} \tag{6.1}$$

Now equation (1.1) gives

$$H_{NR}(\underset{\sim}{\rho}) = \sum_{i=1}^{N} (\frac{\underset{\sim}{p}_i^2}{2} - \frac{1}{\rho_i}) + \frac{1}{Z} \sum_{i<j} \frac{1}{\rho_{ij}} \tag{6.2}$$

with momentum operator $\underset{\sim}{p}_i$ acting in $\underset{\sim}{\rho}$-space. We therefore have

$$H_{NR} = H_{HO} + \tfrac{1}{2} \sum_i (\underset{\sim}{\rho}_i^2 - \frac{1}{\rho_i}) + \frac{1}{Z} \sum_{i<j} \frac{1}{\rho_{ij}}$$

giving us the perturbation potential as

$$V = \tfrac{1}{2} \sum_i (\underset{\sim}{\rho}_i^2 - \frac{1}{\rho_i}) + \frac{1}{Z} \sum_{i<j} \frac{1}{\rho_{ij}}$$

The perturbation expansion is obtained by using the functions $\Phi(\frac{\underset{\sim}{r}}{Z})$, or equivalently $\Psi(\underset{\sim}{r})$ for $Z = 1$, giving the entire Z-dependence in V. We now readily see that a Z-expansion, in decreasing powers, results but since V is a sum of a

Z-dependent term and a term inversely proportional to Z the n^{th}-order correction will contribute to the $E_0, E_1, E_2 \ldots E_n$ terms in the Z-expansion for E. No term can ever be completely determined, whereas in the hydrogenic approximation we can calculate each term by means of a particular order of perturbation theory.

The non-relativistic Z-expansion (1.11) also follows from the change of scale $\underset{\sim}{r} = Z\underset{\sim}{\rho}$ [59].

6.4 RELATIVISTIC CORRECTIONS

The major relativistic corrections are contained in the spin-orbit operator, matrix elements of which are proportional to Z^4 in the hydrogenic approximation. When we add the first-order spin-orbit correction to E2 discussed in chapter 5, we obtain a fine structure ten times larger than observed for CI. This is not surprising since we have assumed that the 2p-electrons are in the field produced by the full nuclear charge of 6 a.u. Full 1s and 2s orbitals are expected to screen the 2p-electrons from the nucleus so that they do not see the entire nuclear charge. If we reduce Z to about 4 a.u. then the first order spin-orbit interaction gives the correct order for the fine structure. Second-order spin-orbit corrections reduce the fine structure till it is five times too big. This correction, as explained in chapter 2, consists of two parts:

1) spin-orbit-spin-orbit corrections

2) Coulomb-spin-orbit corrections.

These depend on Z^6 and Z^3 respectively. Despite the stronger dependence on Z we found that for CI the first of these corrections was a thousand times smaller than the second. It seems reasonable to expect the Coulomb^{n-1}-spin-orbit, and

permutations of these n operators, to be the largest part of the n^{th}-order relativistic correction for atoms and ions at the beginning of an isoelectronic sequence.

Third-order is expected to play a big part in the fine structure calculation since it is the first time that the core orbitals can be opened to allow the p-electrons to see a less heavily screened nucleus. There are several hundred possible species of $Coulomb^2$-spin-orbit excitation sequences making the total number of third-order effective operators rather formidable. Restricting to single-particle excitations for the Coulomb part would give the major third-order correction reducing the number of effective operators down to about ten. Development of new computer languages may make programming of the few identities required for recoupling of the unit tensor operators possible so that the necessary rearrangement of these operators can be done by machine. Until this, the effective operator approach seems unsuitable.

6.5 SUMMARY

This work has shown that the sum over discrete states in evaluating E_2 of Layzer's Z-expansion can be approximated by the first few terms of a small number of different species of perturbing configurations since the convergence of this sum is quite rapid. Continuum states are still causing difficulty because the required Coulomb integrals have not been analytically evaluated.

Fine structure calculations do not appear to be easily obtained by this method as the spin-orbit matrix elements have a very strong dependence on the nuclear charge giving rise to a Z-expansion in increasing powers of Z.

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APPENDIX A

Second-order effective operators for perturbation $\sum_{i<j} \frac{1}{r_{ij}} + \frac{1}{2c^2} \sum_i \frac{1}{r_i^3} (\underset{\sim}{s}_i^{(1)} . \underset{\sim}{\ell}_i^{(1)})$ acting in the ground complex of configurations ℓ^N and $\ell' {}^4\ell' \ell^{N+2}$ with an open n = 2.

Second Order Coulomb-Coulomb Operators Acting in Configuration ℓ^N

$\ell'^{4\ell'}\ell^N\ell''^2$

$$2\sum_K P(KK,\ell'\ell'\ell''\ell'')/[K] - \sum_K(-)^K[K]M(K,\ell'\ell'\ell''\ell'')$$

$\ell'^{4\ell'}\ell^N\ell''\ell'''$

$$4\sum_K P(KK,\ell'\ell'\ell''\ell''')/[K] - 2\sum_K (-)^K[K]M(K,\ell'\ell'\ell''\ell''')$$

$\ell'^{4\ell'}\ell^{N+1}\ell''$

$$4\sum_K P(KK,\ell'\ell'\ell\ell'')/[K] - 2\sum_K (-)^K[K]M(K,\ell'\ell'\ell\ell'')$$

$\ell'^{4\ell'}\ell^{N+2}$

$$\tfrac{1}{2}\sum_K (-)^K[K]M(K,\ell\ell\ell'\ell')\left\{\sum'_{ij}(\underline{u}_i^{(K)}\cdot\underline{u}_j^{(K)}) - 2\frac{[\ell]-N}{[\ell]}\right\} + 2\frac{[\ell]-N}{[\ell]}\sum_K P(KK,\ell\ell\ell'\ell')/[K]$$

$\ell'^{4\ell'+1}\ell''^{4\ell''+1}\ell^N\ell'''^2$

$$4\sum_K P(KK,\ell'\ell''\ell'''\ell''')/[K]$$

$\ell'^{4\ell'+1}\ell''^{4\ell''+1}\ell^N\ell'''\ell''''$

$$4\sum_K \{P(KK,\ell'\ell''\ell'''\ell'''') + P(KK,\ell'\ell''\ell''''\ell''')\}/[K]$$
$$- 4\sum_{KK'}(-)^{K+K'}\ x(K,\ell'\ell''\ell'''\ell'''')\ \ x(K',\ell'\ell''\ell''''\ell''')\begin{Bmatrix} K & \ell'' & \ell''' \\ K' & \ell' & \ell'''' \end{Bmatrix}$$

$\ell'^{4\ell'+1}\ell''^{4\ell''+1}\ell^{N+1}\ell'''$

$$4\sum_K \{P(KK,\ell'\ell''\ell\ell''') + P(KK,\ell'\ell''\ell'''\ell)\}/[K]$$
$$- 4\sum_{KK'}(-)^{K+K'}\ x(K,\ell'\ell''\ell\ell''')\ x\ (K',\ell'\ell''\ell'''\ell)\begin{Bmatrix} K & \ell'' & \ell''' \\ K' & \ell' & \ell \end{Bmatrix}$$

$\ell'^{4\ell'+1}\ell''^{4\ell''+1}\ell^{N+2}$

$$\frac{1}{2}\sum_{K}(-)^{K}[K]M(K,\ell\ell\ell'\ell'')\left\{\sum_{ij}'(\underline{u}_i^{(K)}.\underline{u}_j^{(K)}) - 2\,\frac{[\ell]-N}{[\ell]}\right\} + 2\,\frac{[\ell]-N}{[\ell]}\sum_{K}P(KK,\ell\ell\ell'\ell'')/[K]$$

$\ell^{N-2}\ell'^{2}$

$$\frac{1}{2}\sum_{K}(-)^{K}[K]M(K,\ell\ell\ell'\ell')\sum_{ij}'(\underline{u}_i^{(K)}.\underline{u}_j^{(K)})$$

$\ell^{N-2}\ell'\ell''$

$$\sum_{K}(-)^{K}[K]M(K,\ell\ell\ell'\ell'')\sum_{ij}'(\underline{u}_i^{(K)}.\underline{u}_j^{(K)})$$

$\ell'^{4\ell'+1}\ell^{N-1}\ell''^{2}$

$$\frac{2N}{[\ell]}\sum_{K}P(KK,\ell'\ell\ell''\ell'')/[K]$$

$\ell'^{4\ell'+1}\ell^{N-1}\ell''\ell'''$

$$\frac{2N}{[\ell]}\sum_{K}\{P(KK,\ell'\ell\ell''\ell''') + P(KK,\ell'\ell\ell'''\ell'')\}/[K]$$

$$-\frac{2N}{[\ell]}\sum_{KK'}(-)^{K+K'}\times(K,\ell'\ell\ell''\ell''')\times(K,\ell'\ell\ell'''\ell'')\begin{Bmatrix}K & \ell' & \ell''\\ K' & \ell & \ell'''\end{Bmatrix}$$

$$\ell^{N-1}\ell' \sum_{KK'K''} [K'']P(KK',\ell\ell\ell\ell') \begin{Bmatrix} K & K' & K'' \\ \ell & \ell & \ell' \end{Bmatrix} \Sigma'_{ijr} \{\underline{u}_i^{(K)}.\underline{u}_j^{(K'')}.\underline{u}_r^{(K')}\}_0^0 + \sum_k (-)^K [K]M(K,\ell\ell\ell\ell') \Sigma'_{ij} (\underline{u}_i^{(K)}.\underline{u}_j^{(K)})$$

$$+ \delta(\ell\ell') 4 \left(\frac{[\ell_1]}{[\ell]}\right)^{\frac{1}{2}} X(0,\ell\ell_1\ell'\ell_1) \sum_K X(K,\ell\ell\ell\ell') \Sigma'_{ij} (\underline{u}_i^{(K)}.\underline{u}_j^{(K)})$$

$$+ \delta(\ell\ell') 4 \frac{[\ell_1,\ell_2]^{\frac{1}{2}}}{[\ell]} X(0,\ell\ell_1\ell'\ell_1) X(0,\ell\ell_2\ell'\ell_2)$$

$$- \delta(\ell\ell') \frac{2}{[\ell]} \sum_{KK'} (-)^{K'} X(K,\ell\ell\ell\ell') X(K',\ell_1\ell\ell'\ell_1) \Sigma'_{ij} (\underline{u}_i^{(K)}.\underline{u}_j^{(K)})$$

$$- (-)^{\ell_1+\ell_2} \delta(\ell\ell') 4N \left(\frac{[\ell_1]}{[\ell]^3}\right)^{\frac{1}{2}} X(0,\ell\ell_1\ell'\ell_1) \sum_K (-)^K X(K,\ell_2\ell'\ell\ell_2)$$

$$+ (-)^{\ell_1+\ell_2} \delta(\ell\ell') \frac{N}{[\ell]^2} \sum_{KK'} X(K,\ell_1\ell\ell'\ell_1) X(K',\ell_2\ell\ell'\ell_2)$$

$\ell,4\ell'+1\,\ell^{N}\ell''$

$$
\begin{aligned}
&2\sum_{K} P(KK,\ell\ell'\ell\ell'')(\underline{U}^{K}.\underline{U}^{K})/[K] - 2\sum_{KK'} X(K,\ell\ell'\ell\ell'')\;X(K',\ell\ell\ell'\ell'')\begin{Bmatrix} K & \ell & \ell \\ K' & \ell' & \ell'' \end{Bmatrix}(\underline{U}^{(K)}.\underline{U}^{(K)})\\
&-\sum_{K}[K]M(K,\ell\ell\ell'\ell'')\sum_{ij}{}'(\underline{u}_i^{(K)}.\underline{u}_j^{(K)}) + \frac{2N}{[\ell]}\sum_{K} P(KK,\ell\ell\ell'\ell'')/[K]\\
&+\delta(\ell'\ell'')\Big\{8N\left(\frac{[\ell']}{[\ell]}\right)^{\frac{1}{2}} X(0,\ell\ell'\ell\ell'')X(0,\ell'\ell'\ell'\ell'') - \frac{4N}{[\ell,\ell']^{\frac{1}{2}}}X(0,\ell\ell'\ell\ell'')\sum_{K}X(K,\ell'\ell'\ell'\ell'')\\
&+8N\left(\frac{[\ell_1]}{[\ell]}\right)^{\frac{1}{2}} X(0,\ell\ell'\ell\ell'')X(0,\ell'\ell_1\ell''\ell_1) - \frac{4N}{[\ell,\ell']^{\frac{1}{2}}}X(0,\ell\ell'\ell\ell'')\sum_{K}(-)^{K}X(K,\ell'\ell_1\ell_1\ell'') + 8[\ell']P(00,\ell'\ell'\ell'\ell'')\\
&-8X(0,\ell'\ell'\ell'\ell'')\sum_{K}X(K,\ell'\ell'\ell'\ell'') + \frac{2}{[\ell']}\sum_{KK'}P(KK',\ell'\ell'\ell'\ell'') + 16[\ell',\ell_1]^{\frac{1}{2}}\;X(0,\ell'\ell'\ell'\ell'')\;X(0,\ell'\ell_1\ell''\ell_1)\\
&-8\left(\frac{[\ell_1]}{[\ell']}\right)^{\frac{1}{2}} X(0,\ell'\ell_1\ell''\ell_1)\sum_{K}X(K,\ell'\ell'\ell'\ell'') - \frac{4N}{[\ell]}X(0,\ell'\ell'\ell'\ell'')\sum_{K}(-)^{K}X(K,\ell'\ell\ell\ell'')\\
&+\frac{2N}{[\ell,\ell']}\sum_{KK'}(-)^{K'}X(K,\ell'\ell'\ell'\ell'')X(K',\ell'\ell\ell\ell'') - 8X(0,\ell'\ell'\ell'\ell'')\sum_{K}(-)^{K}X(K,\ell'\ell_1\ell_1\ell'')\\
&+\frac{4}{[\ell']}\sum_{KK'}(-)^{K'}X(K,\ell'\ell'\ell'\ell'')\;X(K',\ell'\ell_1\ell_1\ell'') - \frac{4N}{[\ell]}\left(\frac{[\ell_1]}{[\ell']}\right)^{\frac{1}{2}}X(0,\ell'\ell_1\ell''\ell_1)\sum_{K}(-)^{K}X(K,\ell'\ell\ell\ell'')\\
&-8\left(\frac{[\ell_1]}{[\ell']}\right)^{\frac{1}{2}} X(0,\ell'\ell_1\ell''\ell_1)\sum_{K}(-)^{K}X(K,\ell'\ell_2\ell_2\ell'') + \frac{2N}{[\ell,\ell']}\sum_{KK'}(-)^{K+K'}X(K,\ell'\ell\ell\ell'')X(K',\ell'\ell_1\ell_1\ell'')\\
&+8[\ell_1,\ell_2]^{\frac{1}{2}}X(0,\ell'\ell_1\ell''\ell_1)\;X(0,\ell'\ell_2\ell''\ell_2) + (-)^{\ell_1+\ell_2}\frac{2}{[\ell']}\sum_{KK'}X(K,\ell'\ell_1\ell_1\ell'')X(K'.\ell'\ell_2\ell_2\ell'')\Big\}
\end{aligned}
$$

Off-diagonal Effective Operators Connecting Configurations ℓ^N and $\ell'^{4}\ell'\,\ell^{N+2}$

$\ell'^{4}\ell'\,\ell^{N}\ell''^{2}$

$$\frac{1}{2}\sum_{KK'K''}(-)^{K''}[K'']\;x(K,\ell'\ell'\ell''\ell'')\;x(K',\ell''\ell''\ell\ell)\begin{Bmatrix}K & K' & K''\\ \ell & \ell' & \ell''\end{Bmatrix}^{2}\Sigma'\left(\underline{U}^{(K'')}(\ell'\ell)\cdot\underline{U}^{(K'')}(\ell'\ell)\right)$$

$\ell'^{4}\ell'\,\ell^{N}\ell''\ell'''$

$$\sum_{KK'K''}(-)^{K''}[K'']\;x(K,\ell'\ell'\ell''\ell''')\;x(K',\ell''\ell'''\ell\ell)\begin{Bmatrix}K & K' & K''\\ \ell & \ell' & \ell''\end{Bmatrix}\begin{Bmatrix}K & K' & K''\\ \ell & \ell' & \ell'''\end{Bmatrix}\Sigma'\left((\underline{U}^{(K'')}(\ell'\ell)\cdot\underline{U}^{(K'')}\right.$$

$\ell'^{4}\ell'\,\ell^{N+1}\ell''$

$$\sum_{K'K''}[K'']\;x(K,\ell\ell'\ell'\ell'')\;x(K',\ell\ell\ell\ell'')\begin{Bmatrix}K & K' & K''\\ \ell & \ell' & \ell''\end{Bmatrix}\left\{\underline{U}^{(K)}(\ell'\ell)\times\underline{U}^{(K'')}(\ell'\ell)\times\underline{U}^{(K')}_{(\ell\ell')}\right\}^{(0)}_{0}$$

$$-\frac{\delta(\ell\ell'')}{[\ell]}\sum_{KK'}(-)^{K}\;x(K,\ell\ell'\ell'\ell'')\;x(K',\ell\ell\ell\ell'')\left(\underline{U}^{(K)}(\ell'\ell)\cdot\underline{U}^{(K)}(\ell'\ell)\right)$$

$$+\delta(\ell\ell'')\,2\left(\frac{[\ell_1]}{[\ell]}\right)^{\frac{1}{2}}x(0,\ell\ell_1\ell''\ell_1)\sum_{K}(-)^{K}\;x(K,\ell\ell'\ell'\ell'')\left(\underline{U}^{(K)}(\ell'\ell)\cdot\underline{U}^{(K)}(\ell'\ell)\right)$$

$$-\frac{(-)^{\ell'}\delta(\ell\ell'')}{[\ell]}\sum_{KK'}x\;(K,\ell\ell'\ell'\ell'')\;x\;(K',\ell\ell_1\ell_1\ell'')\left(\underline{U}^{(K)}(\ell'\ell)\cdot\underline{U}^{(K)}(\ell'\ell)\right)$$

$\ell' 4\ell'+1 \ell^N \ell''$

$$\sum_{KK'K''} (-)^{K'} [K''] \times (K, \ell'\ell\ell''\ell) \times (K', \ell'\ell''\ell\ell) \begin{Bmatrix} K & K' & K'' \\ \ell & \ell' & \ell'' \end{Bmatrix} \left\{ \underline{U}^{(K)} \times \underline{U}^{(K'')}(\ell'\ell) \times \underline{U}^{(K')}(\ell'\ell) \right\}_0^{(0)}$$

$$+ \sum_{KK'K''} (-)^{K'} [K''] \times (K, \ell'\ell'\ell''\ell') \times (K', \ell'\ell''\ell\ell) \begin{Bmatrix} K & K' & K'' \\ \ell & \ell' & \ell'' \end{Bmatrix} \left\{ \underline{U}^{(K)}(\ell'\ell') \times \underline{U}^{(K'')}(\ell'\ell) \times \underline{U}^{(K')} \right.$$

$$+ \sum_{KK'K''} (-)^{K''} [K''] \times (K, \ell'\ell\ell\ell'') \times (K', \ell'\ell''\ell\ell) \begin{Bmatrix} K & K' & K'' \\ \ell & \ell & \ell'' \end{Bmatrix} \left\{ \underline{U}^{(K'')} \times \underline{U}^{(K)}(\ell'\ell) \times \underline{U}^{(K')}(\ell'\ell) \right\}_0^{(0)}$$

$$- \frac{\delta(\ell'\ell'')}{[\ell']} \sum_{KK'} (-)^{K'} \times (K, \ell'\ell'\ell''\ell') \times (K', \ell'\ell''\ell\ell) \left(\underline{U}^{(K')}(\ell'\ell) \cdot \underline{U}^{(K')}(\ell'\ell) \right)$$

$$+ \delta(\ell'\ell'') \; 2 \; \times (0, \ell'\ell_1\ell''\ell_1) \sum_{K} \times (K, \ell'\ell''\ell\ell) \left(\underline{U}^{(K)}(\ell'\ell) \cdot \underline{U}^{(K)}(\ell'\ell) \right)$$

Second-order Coulomb-Spin-Orbit Effective Operator Acting in Configuration ℓ^N

$\ell^{N-1}\ell'$

$$[\ell(\ell+1)(2\ell+1)]^{\frac{1}{2}}\xi_{n\ell;n'\ell}\sum_{Kt} x\,(K,\ell\ell\ell\ell')[t]\begin{Bmatrix}1 & K & t\\ \ell & \ell & \ell\end{Bmatrix}\sum_{ij}\{\underline{s}_i^{(1)}\times\underline{u}_i^{(t)}\times\underline{u}_j^{(K)}\}_0^{(0)}$$

$$-\frac{\xi_{n\ell,n'\ell}}{[\ell]}\sum_K x\,(K,\ell\ell\ell\ell')\sum_i(\underline{s}_i^{(1)}\cdot\underline{\ell}_i^{(1)})+2\left(\frac{[\ell_1]}{[\ell]}\right)^{\frac{1}{2}}\xi_{n\ell,n'\ell}\,x\,(0,\ell'\ell_1\ell\ell_1)\sum_i(\underline{s}_i^{(1)}\cdot\underline{\ell}_i^{(1)})$$

$$-(-)^{\ell+\ell_1}\frac{\xi_{n\ell,n'\ell}}{[\ell]}\sum_K x\,(K,\ell'\ell_1\ell_1\ell)\sum_i(\underline{s}_i^{(1)}\cdot\underline{\ell}_i^{(1)})$$

Second-order Spin-orbit-spin-orbit Effective Operator Acting in Configuration ℓ^N

$\ell^{N-1}\ell'$

$$\frac{\xi^2_{n\ell,n'\ell}}{2}\left\{\frac{N\ell(\ell+1)}{2}-\sum_i(\underline{s}_i^{(1)}\cdot\underline{\ell}_i^{(1)})\right\}$$

Off-diagonal Coulomb-spin-orbit Effective Operators Connecting Configurations ℓ^N and $\ell'^4\ell'\,\ell^{N+2}$

$$\ell'^4\ell'\,\ell^{N+1}\ell'' \qquad \delta(\ell\ell'')[\ell(\ell+1)(2\ell+1)]^{\frac{1}{2}}\,\xi_{n\ell,n''\ell}\sum_{kt} x(k,\ell'\ell'\ell\ell'')[t]\begin{Bmatrix} k & 1 & t \\ \ell & \ell' & \ell \end{Bmatrix}\sum_{ij}\{\underline{u}_i^{(t)}(\ell'\ell)\times\underline{s}_j^{(1)}\times\underline{u}_j^{(k)}(\ell'\ell)\}_0^{(0)}$$

APPENDIX B

Zero-order energy, first and second order energy corrections, and the energy difference ratio for both configurations in the ground complex of CI.

NUCLEAR CHARGE=6 (CARBON 1)

ZERO ORDER ENERGY
FIRST ORDER

SECOND ORDER TERMS

	TERM	CORRECTIONS TO $1s^2 2s^2 2p^2$	CORRECTIONS TO $1s^2 2p^4$	ENERGY DIFFERENCE RATIOS $1s^2 2s^2 2p^2$	ENERGY DIFFERENCE RATIOS $1s^2 2p^4$
		-11851626.4			
1S2 2S2 3S2	1S	4349151.9	4741891.3		
	3P	4291427.7	4663729.3		
	1D	4319204.9	4688506.5	1.0781	1.9219
1S2 2S2 3P2	1S	-44.9	-1.9	1.0765	1.9218
1S2 2S2 3S 3D	1S	-316.2	-13.2		
	3P	-91.3	-1.8		
	1D	-167.8	-1.9	1.0741	1.9215
1S2 2S2 3D2	1D	-43.7	-0.5	1.0774	1.9215
1S2 2S2 3S 4S	1S	-1068.1	-44.5		
	3P	-245.5	-2.7		
	1D	-249.7	-2.8	1.0480	1.9200
1S2 2S2 3D 4S	1S	-25.5	-1.1	1.0475	1.9200
1S2 2S2 3P 4P	1D	-8.6	-0.1	1.0477	1.9200
1S2 2S2 3S 4D	1S	-171.4	-7.1		
	3P	-47.1	-0.5		
	1D	-88.9	-1.0	1.0463	1.9198
1S2 2S2 3D 4D	1D	-18.9	-0.2	1.0477	1.9198
1S2 2S2 3P 4F	1S	-566.3	-23.5		
	3P	-127.5	-1.4		
	1D	-131.6	-1.5	1.0321	1.9191
1S2 2S2 4S2	1D	-3.3	-0.0	1.0321	1.9190
1S2 2S2 4P2	1S	-3.9	-0.2	1.0319	1.9191
1S2 2S2 4S 4D	1S	-25.5	-1.1		
	3P	-6.4	-0.1		
	1D	-12.8	-0.1	1.0317	1.9190
1S2 2S2 4D2	1D	-4.2	-0.0	1.0320	1.9190
	1S	-83.9	-3.5		
	3P	-18.1	-0.2		
	1D	-19.2	-0.2	1.0297	1.9189

1S2 2S2 4P 4F				
1S2 2S2 4F2	1D	-0.2	-0.0	1.0297	1.9189
	1S	-3.4	-0.1		
	3P	-0.4	-0.0		
	1D	-0.6	-0.0	1.0296	1.9189
1S2 2S2 3S 5S	1S	-10.9	-0.5	1.0293	1.9189
1S2 2S2 3D 5S	1D	-3.1	-0.0	1.0295	1.9189
1S2 2S2 3P 5P	1S	-71.7	-3.0		
	3P	-19.5	-0.2		
	1D	-37.0	-0.4	1.0289	1.9188
1S2 2S2 3S 5D	1D	-9.4	-0.1	1.0296	1.9188
1S2 2S2 3D 5D	1S	-234.0	-9.7		
	3P	-52.6	-0.6		
	1D	-54.3	-0.6	1.0231	1.9185
1S2 2S2 3P 5F	1D	-0.1	-0.0	1.0231	1.9185
1S2 2S2 4S 5S	1S	-3.5	-0.1	1.0230	1.9185
1S2 2S2 4D 5S	1D	-1.6	-0.0	1.0231	1.9185
1S2 2S2 4P 5P	1S	-22.2	-0.9		
	3P	-5.5	-0.1		
	1D	-11.0	-0.1	1.0229	1.9185
1S2 2S2 4F 5P	1D	-0.1	-0.0	1.0229	1.9185
1S2 2S2 4S 5D	1D	-2.2	-0.0	1.0231	1.9185
1S2 2S2 4D 5D	1S	-72.5	-3.0		
	3P	-15.4	-0.2		
	1D	-16.6	-0.2	1.0211	1.9184
1S2 2S2 4P 5F	1D	-0.1	-0.0	1.0211	1.9184
1S2 2S2 4F 5F	1S	-4.0	-0.2		
	3P	-0.5	-0.0		
	1D	-0.7	-0.0	1.0210	1.9184
1S2 2S2 5S2	1S	-0.8	-0.0	1.0210	1.9183
1S2 2S2 5P2	1S	-4.9	-0.2		
	3P	-1.2	-0.0		
	1D	-2.4	-0.0	1.0209	1.9183

1S2 2S2 5S 5D					
1S2 2S2 5D2	1D	-0.9	-0.0	1.0210	1.9183
	1S	-15.9	-0.7		
	3P	-3.3	-0.3		
	1D	-3.6	-0.0	1.0205	1.9183
1S2 2S2 5P 5F					
1S2 2S2 5F2	1D	-0.1	-0.0	1.0205	1.9183
	1S	-1.2	-0.0		
	3P	-0.2	-0.0		
	1D	-0.2	-0.0	1.0205	1.9183
2S2 2P4					
	1S	-1930.1	-79.3		
	3P	-1242.1	-13.8		
	1D	-1242.1	-13.7	0.9955	1.9160
1S 2S2 2P2 3S					
	1S	-10638.7	-423.1		
	3P	-10985.0	-117.8		
	1D	-10944.6	-117.2	1.0051	1.9049
1S 2S2 2P2 3D					
	1S	-31.4	-1.2		
	3P	-163.5	-1.7		
	1D	-185.6	-1.9	1.0116	1.9049
1S 2S2 2P2 4S					
	1S	-3896.8	-149.3		
	3P	-4018.1	-41.4		
	1D	-4004.9	-41.2	1.0150	1.9010
1S 2S2 2P2 4D					
	1S	-9.1	-0.3		
	3P	-61.6	-0.6		
	1D	-69.2	-0.7	1.0175	1.9011
1S 2S2 2P2 5S					
	1S	-1873.2	-70.7		
	3P	-1930.5	-19.6		
	1D	-1924.5	-19.5	1.0191	1.8992
1S 2S2 2P2 5D					
	1S	-3.8	-0.1		
	3P	-29.7	-0.3		
	1D	-33.2	-0.3	1.0203	1.8992
1S 2S2 2P2 6S					
	1S	-1048.1	-39.3		
	3P	-1079.9	-10.9		
	1D	-1076.6	-10.8	1.0212	1.8982
1S 2S2 2P2 6D					
	1S	-2.0	-0.1		
	3P	-16.6	-0.2		
	1D	-18.6	-0.2	1.0219	1.8982
1S 2S2 2P2 7S					
	1S	-646.9	-24.1		
	3P	-666.4	-6.7		
	1D	-664.4	-6.6	1.0224	1.8976

1S 2S2 2P2 7D	1S	-1.2	-0.0		
	3P	-10.3	-0.1		
	1D	-11.4	-0.1	1.0228	1.8976
1S 2S2 2P2 8S	1S	-427.8	-15.9		
	3P	-440.6	-4.4		
	1D	-439.3	-4.4	1.0232	1.8972
1S 2S2 2P2 8D	1S	-0.8	-0.0		
	3P	-6.8	-0.1		
	1D	-7.6	-0.1	1.0235	1.8972
1S 2S2 2P2 9S	1S	-297.8	-11.1		
	3P	-306.7	-3.1		
	1D	-305.8	-3.0	1.0237	1.8969
1S 2S2 2P2 9D	1S	-0.5	-0.0		
	3P	-4.7	-0.0		
	1D	-5.3	-0.1	1.0239	1.8969
1S 2S2 2P2 10S	1S	-215.7	-8.0		
	3P	-222.2	-2.2		
	1D	-221.5	-2.2	1.0241	1.8967
1S 2S2 2P2 10D	1S	-0.4	-0.0		
	3P	-3.4	-0.0		
	1D	-3.8	-0.0	1.0243	1.8967
1S2 2S 2P2 3S	1S	-183356.0	-10624.7		
	3P	-195097.6	1427.2		
	1D	-195338.0	2288.4	1.4720	1.3887
1S2 2S 2P2 3D	1S	-4329.0	3.8		
	3P	-3120.9	-6609.4		
	1D	-3034.1	-9723.6	1.4201	1.9393
1S2 2S 2P2 4S	1S	-38629.7	-1840.5		
	3P	-40676.3	267.8		
	1D	-40697.7	412.7	1.4967	1.8405
1S2 2S 2P2 4D	1S	-1134.1	56.8		
	3P	-859.9	-1564.0		
	1D	-857.1	-2320.9	1.4865	1.9919
1S2 2S 2P2 5S	1S	-14988.6	-686.6		
	3P	-15749.7	97.7		
	1D	-15756.2	150.4	1.5149	1.9542
1S2 2S 2P2 5D	1S	-463.5	23.1		
	3P	-360.3	-630.6		
	1D	-360.9	-938.4	1.5111	2.0176

1S2 2S 2P2 6S	1S	-7531.9	-338.4		
	3P	-7906.4	47.5		
	1D	-7909.4	73.2	1.5251	1.9988
1S2 2S 2P2 6D	1S	-237.6	11.1		
	3P	-187.2	-322.3		
	1D	-187.8	-480.2	1.5233	2.0317
1S2 2S 2P2 7S	1S	-4368.7	-194.0		
	3P	-4583.2	27.0		
	1D	-4584.9	41.7	1.5313	2.0209
1S2 2S 2P2 7D	1S	-139.1	6.1		
	3P	-110.5	-188.6		
	1D	-111.0	-281.3	1.5303	2.0403
1S2 2S 2P2 8S	1S	-2777.6	-122.4		
	3P	-2912.9	17.0		
	1D	-2914.0	26.2	1.5353	2.0334
1S2 2S 2P2 8D	1S	-88.9	3.7		
	3P	-71.0	-120.6		
	1D	-71.3	-179.9	1.5347	2.0459
1S2 2S 2P2 9S	1S	-1883.0	-82.6		
	3P	-1974.3	11.4		
	1D	-1975.0	17.6	1.5381	2.0413
1S2 2S 2P2 9D	1S	-60.5	2.5		
	3P	-48.5	-82.0		
	1D	-48.7	-122.4	1.5377	2.0498
1S2 2S 2P2 10S	1S	-1338.8	-58.5		
	3P	-1403.4	8.1		
	1D	-1403.9	12.4	1.5401	2.0465
1S2 2S 2P2 10D	1S	-43.1	1.7		
	3P	-34.6	-58.5		
	1D	-34.8	-87.2	1.5398	2.0526
1S2 2S2 2P 3P	1S	-211819.4	-2224.1		
	3P	-189069.8	-667.5		
	1D	-198497.1	-787.0	1.6064	2.0034
1S2 2S2 2P 4P	1S	-43787.6	-330.6		
	3P	-39614.2	-103.7		
	1D	-41330.5	-119.8	1.6249	1.9960
1S2 2S2 2P 4F	1D	-49.0	-0.1	1.6328	1.9960

1S2 2S2 2P 5P					
	1S	-16838.7	-118.8		
	3P	-15352.1	-37.7		
	1D	-15964.4	-43.3	1.6409	1.9934
1S2 2S2 2P 5F					
	1D	-30.5	-0.1	1.6461	1.9934
1S2 2S2 2P 6P					
	1S	-8417.5	-57.8		
	3P	-7708.3	-18.5		
	1D	-8000.9	-21.2	1.6504	1.9921
1S2 2S2 2P 6F					
	1D	-18.8	-0.0	1.6536	1.9921
1S2 2S2 2P 7P					
	1S	-4866.3	-32.9		
	3P	-4468.5	-10.6		
	1D	-4632.8	-12.1	1.6562	1.9913
1S2 2S2 2P 7F					
	1D	-12.1	-0.0	1.6583	1.9913
1S2 2S2 2P 8P					
	1S	-3087.3	-20.7		
	3P	-2840.0	-6.7		
	1D	-2942.2	-7.6	1.6599	1.9909
1S2 2S2 2P 8F					
	1D	-8.3	-0.0	1.6614	1.9909
1S2 2S2 2P 9P					
	1S	-2089.8	-13.9		
	3P	-1924.8	-4.5		
	1D	-1993.0	-5.1	1.6625	1.9906
1S2 2S2 2P 9F					
	1D	-5.8	-0.0	1.6636	1.9906
1S2 2S2 2P 10P					
	1S	-1484.1	-9.9		
	3P	-1368.2	-3.2		
	1D	-1416.1	-3.6	1.6644	1.9904
1S2 2S2 2P 10F					
	1D	-4.3	-0.0	1.6651	1.9904
2S2 2P2 3S2					
	1S	-8.2	-0.1		
	3P	-8.2	-0.0		
	1D	-8.2	-0.0	1.6652	1.9904
2S2 2P2 3P2					
	1S	-15.1	-0.1		
	3P	-15.2	-0.0		
	1D	-15.2	-0.0	1.6652	1.9904
2S2 2P2 3S 3D					
	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	1.6652	1.9904
2S2 2P2 3D2					
	1S	-0.1	-0.0		
	3P	-0.1	-0.0		
	1D	-0.1	-0.0	1.6652	1.9904

2S2 2P2 3S 4S	1S	-6.4	-0.0		
	3P	-6.5	-0.0		
	1D	-6.5	-0.0	1.6652	1.9904
2S2 2P2 3D 4S	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	1.6652	1.9904
2S2 2P2 3P 4P	1S	-12.0	-0.1		
	3P	-12.0	-0.0		
	1D	-12.0	-0.0	1.6652	1.9904
2S2 2P2 3S 4D	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	1.6652	1.9904
2S2 2P2 3D 4D	1S	-0.1	-0.0		
	3P	-0.1	-0.0		
	1D	-0.1	-0.0	1.6652	1.9904
2S2 2P2 3P 4F	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	1.6652	1.9904
2S2 2P2 4S2	1S	-1.3	-0.0		
	3P	-1.3	-0.0		
	1D	-1.3	-0.0	1.6652	1.9904
2S2 2P2 4P2	1S	-2.4	-0.0		
	3P	-2.4	-0.0		
	1D	-2.4	-0.0	1.6652	1.9904
2S2 2P2 4S 4D	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	1.6652	1.9904
2S2 2P2 4D2	1S	-0.0	-0.0		
	3P	-0.0	-0.0		
	1D	-0.0	-0.0	1.6652	1.9904
2S2 2P2 4P 4F	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	1.6652	1.9904
2S2 2P2 4F2	1S	-0.0	-0.0		
	3P	-0.0	-0.0		
	1D	-0.0	-0.0	1.6652	1.9904
2S2 2P2 3S 5S	1S	-3.2	-0.0		
	3P	-3.2	-0.0		
	1D	-3.2	-0.0	1.6652	1.9904

2S2 2P2 3D 5S	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	1.6652	1.9904
2S2 2P2 3P 5P	1S	-5.9	-0.0		
	3P	-6.0	-0.0		
	1D	-6.0	-0.0	1.6652	1.9904
2S2 2P2 3S 5D	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	1.6652	1.9904
2S2 2P2 3D 5D	1S	-0.0	-0.0		
	3P	-0.0	-0.0		
	1D	-0.0	-0.0	1.6652	1.9904
2S2 2P2 3P 5F	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	1.6652	1.9904
2S2 2P2 4S 5S	1S	-1.3	-0.0		
	3P	-1.3	-0.0		
	1D	-1.3	-0.0	1.6652	1.9903
2S2 2P2 4D 5S	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	1.6652	1.9903
2S2 2P2 4P 5P	1S	-2.4	-0.0		
	3P	-2.4	-0.0		
	1D	-2.4	-0.0	1.6652	1.9903
2S2 2P2 4F 5P	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	1.6652	1.9903
2S2 2P2 4S 5D	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	1.6652	1.9903
2S2 2P2 4D 5D	1S	-0.0	-0.0		
	3P	-0.0	-0.0		
	1D	-0.0	-0.0	1.6652	1.9903
2S2 2P2 4P 5F	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	1.6652	1.9903
2S2 2P2 4F 5F	1S	-0.0	-0.0		
	3P	-0.0	-0.0		
	1D	-0.0	-0.0	1.6652	1.9903

2S2 2P2 5S2	1S	-0.3	-0.0		
	3P	-0.3	-0.0		
	1D	-0.3	-0.0	1.6652	1.9903
2S2 2P2 5P2	1S	-0.6	-0.0		
	3P	-0.6	-0.0		
	1D	-0.6	-0.0	1.6652	1.9903
2S2 2P2 5S 5D	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	1.6652	1.9903
2S2 2P2 5D2	1S	-0.0	-0.0		
	3P	-0.0	-0.0		
	1D	-0.0	-0.0	1.6652	1.9903
2S2 2P2 5P 5F	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	1.6652	1.9903
2S2 2P2 5F2	1S	-0.0	-0.0		
	3P	-0.0	-0.0		
	1D	-0.0	-0.0	1.6652	1.9903
1S2 2P2 3S2	1S	-100.2	-50.5		
	3P	-82.0	-21.9		
	1D	-79.8	-24.1	1.6635	1.9894
1S2 2P2 3P2	1S	-65.3	-971.7		
	3P	-28.9	-771.0		
	1D	-25.5	-851.8	1.6605	1.9911
1S2 2P2 3S 3D	1S	-0.5	-73.2		
	3P	-0.2	-73.5		
	1D	-0.3	-117.5	1.6605	1.9966
1S2 2P2 3D2	1S	-565.8	-2505.0		
	3P	-359.5	-1846.9		
	1D	-336.9	-1873.7	1.6425	1.9726
1S2 2P2 3S 4S	1S	-53.2	-28.8		
	3P	-43.2	-12.3		
	1D	-42.1	-13.4	1.6416	1.9720
1S2 2P2 3D 4S	1S	-0.1	-14.4		
	3P	-0.0	-14.4		
	1D	-0.1	-23.1	1.6416	1.9731
1S2 2P2 3P 4P	1S	-35.1	-515.8		
	3P	-15.4	-404.6		
	1D	-13.6	-448.7	1.6400	1.9740

1S2 2P2 3S 4D	1S	-0.2	-31.7		
	3P	-0.1	-31.8		
	1D	-0.1	-50.9	1.6400	1.9763
1S2 2P2 3D 4D	1S	-266.0	-1322.0		
	3P	-163.2	-963.9		
	1D	-152.3	-978.9	1.6311	1.9632
1S2 2P2 3P 4F	1S	-0.0	-0.6		
	3P	-0.0	-0.6		
	1D	-0.0	-0.9	1.6311	1.9633
1S2 2P2 4S2	1S	-7.7	-4.5		
	3P	-6.2	-1.9		
	1D	-6.0	-2.0	1.6310	1.9632
1S2 2P2 4P2	1S	-5.7	-74.2		
	3P	-2.6	-57.2		
	1D	-2.3	-63.9	1.6307	1.9633
1S2 2P2 4S 4D	1S	-0.0	-7.0		
	3P	-0.0	-7.0		
	1D	-0.0	-11.2	1.6307	1.9638
1S2 2P2 4D2	1S	-36.4	-193.4		
	3P	-21.8	-138.8		
	1D	-20.3	-141.6	1.6295	1.9619
1S2 2P2 4P 4F	1S	-0.0	-0.4		
	3P	-0.0	-0.4		
	1D	-0.0	-0.6	1.6295	1.9619
1S2 2P2 4F2	1S	-3.3	-6.4		
	3P	-2.4	-4.2		
	1D	-2.3	-4.4	1.6294	1.9619
1S2 2P2 3S 5S	1S	-22.2	-12.3		
	3P	-18.0	-5.2		
	1D	-17.5	-5.7	1.6290	1.9616
1S2 2P2 3D 5S	1S	-0.0	-5.3		
	3P	-0.0	-5.3		
	1D	-0.0	-8.5	1.6290	1.9620
1S2 2P2 3P 5P	1S	-14.3	-214.9		
	3P	-6.1	-168.1		
	1D	-5.4	-186.6	1.6283	1.9623
1S2 2P2 3S 5D	1S	-0.1	-15.8		
	3P	-0.0	-15.8		
	1D	-0.1	-25.3	1.6283	1.9635

1S2 2P2 3D 5D	1S	-103.3	-546.6		
	3P	-62.2	-397.2		
	1D	-57.9	-403.3	1.6248	1.9580
1S2 2P2 3P 5F	1S	-0.0	-0.2		
	3P	-0.0	-0.2		
	1D	-0.0	-0.3	1.6248	1.9580
1S2 2P2 4S 5S	1S	-6.6	-4.0		
	3P	-5.3	-1.6		
	1D	-5.2	-1.8	1.6247	1.9580
1S2 2P2 4D 5S	1S	-0.0	-2.7		
	3P	-0.0	-2.7		
	1D	-0.0	-4.3	1.6247	1.9582
1S2 2P2 4P 5P	1S	-5.0	-63.9		
	3P	-2.3	-49.0		
	1D	-2.0	-54.8	1.6245	1.9583
1S2 2P2 4F 5P	1S	-0.0	-0.2		
	3P	-0.0	-0.2		
	1D	-0.0	-0.3	1.6245	1.9583
1S2 2P2 4S 5D	1S	-0.0	-3.6		
	3P	-0.0	-3.7		
	1D	-0.0	-5.9	1.6245	1.9585
1S2 2P2 4D 5D	1S	-30.1	-166.5		
	3P	-17.8	-119.0		
	1D	-16.5	-121.4	1.6234	1.9569
1S2 2P2 4P 5F	1S	-0.0	-0.2		
	3P	-0.0	-0.2		
	1D	-0.0	-0.3	1.6234	1.9569
1S2 2P2 4F 5F	1S	-3.7	-7.5		
	3P	-2.7	-4.9		
	1D	-2.6	-5.1	1.6233	1.9568
1S2 2P2 5S2	1S	-1.5	-0.9		
	3P	-1.2	-0.4		
	1D	-1.1	-0.4	1.6233	1.9568
1S2 2P2 5P2	1S	-1.1	-13.9		
	3P	-0.5	-10.6		
	1D	-0.5	-11.9	1.6232	1.9568
1S2 2P2 5S 5D	1S	-0.0	-1.4		
	3P	-0.0	-1.4		
	1D	-0.0	-2.3	1.6232	1.9569

1S2 2P2 5D2					
	1S	-6.4	-36.5		
	3P	-3.7	-25.9		
	1D	-3.5	-26.5	1.6230	1.9565
1S2 2P2 5P 5F					
	1S	-0.0	-0.1		
	3P	-0.0	-0.1		
	1D	-0.0	-0.2	1.6230	1.9565
1S2 2P2 5F2					
	1S	-1.1	-2.3		
	3P	-0.8	-1.5		
	1D	-0.7	-1.5	1.6230	1.9565
2S2 2P3 3P					
	1S	-122.2	-0.9		
	3P	-122.8	-0.3		
	1D	-122.8	-0.3	1.6230	1.9565
2S2 2P3 4P					
	1S	-47.9	-0.3		
	3P	-48.2	-0.1		
	1D	-48.2	-0.1	1.6230	1.9565
2S2 2P3 4F					
	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	1.6230	1.9565
2S2 2P3 5P					
	1S	-23.7	-0.2		
	3P	-23.8	-0.1		
	1D	-23.8	-0.1	1.6230	1.9565
2S2 2P3 5F					
	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	1.6230	1.9565
1S2 2P3 3P					
	1S	-6577.4	-459403.9		
	3P	-1714.9	-438729.1		
	1D	-1895.4	-448587.8	1.3240	2.5608
1S2 2P3 4P					
	1S	-3660.7	-92726.2		
	3P	-674.0	-91086.1		
	1D	-703.3	-92879.8	1.1247	2.9491
1S2 2P3 4F					
	1S	0.0	0.0		
	3P	-0.5	-40.5		
	1D	-0.9	-72.8	1.1248	2.9628
1S2 2P3 5P					
	1S	-1979.0	-35126.3		
	3P	-324.9	-35131.7		
	1D	-330.7	-35776.3	1.0126	3.1845
1S2 2P3 5F					
	1S	0.0	0.0		
	3P	-0.3	-25.2		
	1D	-0.7	-45.2	1.0127	3.1939

1S 2S 2P4	1S	-928.8	153.9		
	3P	-379.2	-105.7		
	1D	-373.9	-111.0	0.9744	3.2183
1S 2S 2P3 3P	1S	-146.1	-7.8		
	3P	-151.9	-2.0		
	1D	-151.7	-2.2	0.9748	3.2179
1S 2S 2P2 3S2	1S	-7.2	-0.4		
	3P	-7.5	-0.1		
	1D	-7.5	-0.1	0.9748	3.2179
1S 2S 2P2 3P2	1S	-2.9	-0.2		
	3P	-3.0	-0.0		
	1D	-3.0	-0.0	0.9748	3.2179
1S 2S 2P2 3S 3D	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	0.9748	3.2179
1S 2S 2P2 3D2	1S	-5.0	-0.3		
	3P	-5.2	-0.1		
	1D	-5.2	-0.1	0.9748	3.2178
1S 2S 2P3 4P	1S	-55.5	-3.0		
	3P	-57.7	-0.8		
	1D	-57.7	-0.8	0.9750	3.2177
1S 2S 2P3 4F	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	0.9750	3.2177
1S 2S 2P2 3S 4S	1S	-2.8	-0.1		
	3P	-2.9	-0.0		
	1D	-2.9	-0.0	0.9750	3.2177
1S 2S 2P2 3D 4S	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	0.9750	3.2177
1S 2S 2P2 3P 4P	1S	-0.8	-0.0		
	3P	-0.9	-0.0		
	1D	-0.9	-0.0	0.9750	3.2177
1S 2S 2P2 3S 4D	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	0.9750	3.2177
1S 2S 2P2 3D 4D	1S	-2.1	-0.1		
	3P	-2.1	-0.0		
	1D	-2.1	-0.0	0.9750	3.2177

1S 2S 2P2 3P 4F				
	1S	0.0	0.0	
	3P	0.0	0.0	
	1D	0.0	0.0	0.9750 3.2177
1S 2S 2P2 4S2				
	1S	-1.0	-0.1	
	3P	-1.1	-0.0	
	1D	-1.1	-0.0	0.9750 3.2177
1S 2S 2P2 4P2				
	1S	-0.1	-0.0	
	3P	-0.1	-0.0	
	1D	-0.1	-0.0	0.9750 3.2177
1S 2S 2P2 4S 4D				
	1S	0.0	0.0	
	3P	0.0	0.0	
	1D	0.0	0.0	0.9750 3.2177
1S 2S 2P2 4D2				
	1S	-0.8	-0.0	
	3P	-0.9	-0.0	
	1D	-0.9	-0.0	0.9750 3.2177
1S 2S 2P2 4P 4F				
	1S	0.0	0.0	
	3P	0.0	0.0	
	1D	0.0	0.0	0.9750 3.2177
1S 2S 2P2 4F2				
	1S	-0.0	-0.0	
	3P	-0.0	-0.0	
	1D	-0.0	-0.0	0.9750 3.2177
1S 2S 2P3 5P				
	1S	-27.2	-1.5	
	3P	-28.3	-0.4	
	1D	-28.3	-0.4	0.9751 3.2176
1S 2S 2P2 3S 5S				
	1S	0.0	0.0	
	3P	0.0	0.0	
	1D	0.0	0.0	0.9751 3.2176
1S 2S 2P2 3D 5S				
	1S	-1.3	-0.1	
	3P	-1.4	-0.0	
	1D	-1.4	-0.0	0.9751 3.2176
1S 2S 2P2 3P 5P				
	1S	0.0	0.0	
	3P	0.0	0.0	
	1D	0.0	0.0	0.9751 3.2176
1S 2S 2P2 3S 5D				
	1S	-0.4	-0.0	
	3P	-0.4	-0.0	
	1D	-0.4	-0.0	0.9751 3.2176
	1S	0.0	0.0	
	3P	0.0	0.0	
	1D	0.0	0.0	0.9751 3.2176

1S 2S 2P2 3D 5D	1S	-1.0	-0.1		
	3P	-1.1	-0.0		
	1D	-1.1	-0.0	0.9751	3.2176
1S 2S 2P2 3P 5F	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	0.9751	3.2176
1S 2S 2P2 4S 5S	1S	-0.5	-0.0		
	3P	-0.5	-0.0		
	1D	-0.5	-0.0	0.9751	3.2176
1S 2S 2P2 4D 5S	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	0.9751	3.2176
1S 2S 2P2 4P 5P	1S	-0.2	-0.0		
	3P	-0.1	-0.0		
	1D	-0.1	-0.0	0.9751	3.2176
1S 2S 2P2 4F 5P	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	0.9751	3.2176
1S 2S 2P2 4S 5D	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	0.9751	3.2176
1S 2S 2P2 4D 5D	1S	-0.4	-0.0		
	3P	-0.4	-0.0		
	1D	-0.4	-0.0	0.9751	3.2176
1S 2S 2P2 4P 5F	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	0.9751	3.2176
1S 2S 2P2 4F 5F	1S	-0.0	-0.0		
	3P	-0.0	-0.0		
	1D	-0.0	-0.0	0.9751	3.2176
1S 2S 2P2 5S2	1S	-0.3	-0.0		
	3P	-0.3	-0.0		
	1D	-0.3	-0.0	0.9751	3.2176
1S 2S 2P2 5P2	1S	-0.0	-0.0		
	3P	-0.0	-0.0		
	1D	-0.0	-0.0	0.9751	3.2176
1S 2S 2P2 5S 5D	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	0.9751	3.2176

1S 2S 2P2 5D2	1S	-0.2	-0.0		
	3P	-0.2	-0.0		
	1D	-0.2	-0.0	0.9751	3.2176
1S 2S 2P2 5P 5F	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	0.9751	3.2176
1S 2S 2P2 5F2	1S	-0.0	-0.0		
	3P	-0.0	-0.0		
	1D	-0.0	-0.0	0.9751	3.2176
1S 2P4 3S	1S	-698.7	-12619.5		
	3P	-178.3	-13181.9		
	1D	-195.2	-13123.0	0.9418	3.2449
1S 2P4 3D	1S	-1.8	-30.8		
	3P	-2.3	-162.9		
	1D	-2.9	-184.7	0.9419	3.2644
1S 2P4 4S	1S	-265.7	-4565.4		
	3P	-68.2	-4776.3		
	1D	-74.7	-4756.4	0.9293	3.2752
1S 2P4 4D	1S	-0.5	-8.9		
	3P	-0.9	-61.4		
	1D	-1.1	-68.8	0.9293	3.2825
1S 2P4 5S	1S	-129.6	-2183.4		
	3P	-33.3	-2285.8		
	1D	-36.5	-2276.4	0.9231	3.2879
1S 2P4 5D	1S	-0.2	-3.8		
	3P	-0.4	-29.6		
	1D	-0.5	-33.0	0.9232	3.2914
1S 2P4 6S	1S	-73.1	-1218.4		
	3P	-18.8	-1276.3		
	1D	-20.6	-1270.9	0.9197	3.2945
1S 2P4 6D	1S	-0.1	-2.0		
	3P	-0.2	-16.6		
	1D	-0.3	-18.4	0.9197	3.2964
1S 2P4 7S	1S	-45.3	-750.8		
	3P	-11.7	-786.5		
	1D	-12.8	-783.3	0.9176	3.2983
1S 2P4 7D	1S	-0.1	-1.2		
	3P	-0.2	-10.2		
	1D	-0.2	-11.4	0.9176	3.2995

1S 2P4 8S					
	1S	-30.0	-496.0		
	3P	-7.7	-519.6		
	1D	-8.5	-517.5	0.9161	3.3008
1S 2P4 8D					
	1S	-0.0	-0.7		
	3P	-0.1	-6.8		
	1D	-0.1	-7.5	0.9161	3.3016
1S 2P4 9S					
	1S	-20.9	-345.0		
	3P	-5.4	-361.5		
	1D	-5.9	-360.1	0.9151	3.3025
1S 2P4 9D					
	1S	-0.0	-0.5		
	3P	-0.1	-4.7		
	1D	-0.1	-5.2	0.9152	3.3030
1S 2P4 10S					
	1S	-15.2	-249.8		
	3P	-3.9	-261.8		
	1D	-4.3	-260.7	0.9144	3.3037
1S 2P4 10D					
	1S	-0.0	-0.4		
	3P	-0.1	-3.4		
	1D	-0.1	-3.8	0.9144	3.3041
2P6					
	1S	4.9	80.4	0.9148	3.3110
2P5 3P					
	1S	-7.1	-116.0		
	3P	-1.8	-121.3		
	1D	-2.0	-121.1	0.9144	3.3114
2P5 4P					
	1S	-2.8	-45.5		
	3P	-0.7	-47.6		
	1D	-0.8	-47.5	0.9143	3.3116
2P5 4F					
	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	0.9143	3.3116
2P5 5P					
	1S	-1.4	-22.5		
	3P	-0.4	-23.5		
	1D	-0.4	-23.5	0.9142	3.3116
2P5 5F					
	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	0.9142	3.3116
2P4 3S2					
	1S	-0.5	-7.7		
	3P	-0.1	-8.1		
	1D	-0.1	-8.1	0.9142	3.3117

2P4 3P2	1S	-0.9	-14.3		
	3P	-0.2	-15.0		
	1D	-0.2	-15.0	0.9142	3.3117
2P4 3S 3D	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	0.9142	3.3117
2P4 3D2	1S	-0.0	-0.1		
	3P	-0.0	-0.1		
	1D	-0.0	-0.1	0.9142	3.3117
2P4 3S 4S	1S	-0.4	-6.1		
	3P	-0.1	-6.4		
	1D	-0.1	-6.4	0.9142	3.3117
2P4 3D 4S	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	0.9142	3.3117
2P4 3P 4P	1S	-0.7	-11.3		
	3P	-0.2	-11.9		
	1D	-0.2	-11.8	0.9141	3.3118
2P4 3S 4D	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	0.9141	3.3118
2P4 3D 4D	1S	-0.0	-0.1		
	3P	-0.0	-0.1		
	1D	-0.0	-0.1	0.9141	3.3118
2P4 3P 4F	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	0.9141	3.3118
2P4 3S 5S	1S	-0.2	-3.0		
	3P	-0.0	-3.2		
	1D	-0.1	-3.2	0.9141	3.3118
2P4 3D 5S	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	0.9141	3.3118
2P4 3P 5P	1S	-0.3	-5.6		
	3P	-0.1	-5.9		
	1D	-0.1	-5.9	0.9141	3.3118
2P4 3S 5D	1S	0.0	0.0		
	3P	0.0	0.0		
	1D	0.0	0.0	0.9141	3.3118

	2P4 3D 5D				
		1S	-0.0	-0.0	
		3P	-0.0	-0.0	
		1D	-0.0	-0.0	0.9141 3.3118
	2P4 3P 5F				
		1S	0.0	0.0	
		3P	0.0	0.0	
		1D	0.0	0.0	0.9141 3.3118
TOTAL ENERGIES			-8096290.9	-7743965.4	
			-8124259.8	-7793924.1	
			-8109647.8	-7782337.5	0.914098 3.311789

APPENDIX C

Z-expansion energies and energy difference ratios, up to second order, for the CI isoelectronic sequence from Z = 6 to Z = 50.

DIAGONALIZED 1/Z ENERGIES (IN CM-1) FOR THE CARBON1 ISOELECTRONIC SEQUENCE

Z	E0	E1	E2	E2(H.F)	(1S-1D)/(1D-3P) E2	E2(H.F)
6	-11851626.	-7502474. -7560199. -7532421.	-8096291. -8124255. -8109642.	-8071396. -8111710. -8096398.	0.914	1.633
7	-16131380.	-11057370. -11124715. -11092308.	-11651098. -11688757. -11669503.	-11624945. -11676160. -11656237.	0.956	1.571
8	-21069558.	-15270699. -15347654. -15310618.	-15864352. -15911686. -15887794.	-15837082. -15899041. -15874506.	0.981	1.525
9	-26666159.	-20142431. -20229018. -20187352.	-20736045. -20793042. -20764513.	-20707780. -20780353. -20751204.	0.998	1.490
10	-32921184.	-25672598. -25768805. -25722509.	-26266173. -26332822. -26299660.	-26237016. -26323094. -26286328.	1.010	1.460
11	-39834633.	-31861188. -31967016. -31916091.	-32454732. -32531028. -32493232.	-32424772. -32518263. -32479880.	1.019	1.436
12	-47406505.	-38708202. -38823650. -38768096.	-39301720. -39387659. -39345229.	-39271035. -39374860. -39331859.	1.025	1.414
13	-55636802.	-46213639. -46338708. -46278524.	-46807136. -46902713. -46855651.	-46775792. -46899885. -46842263.	1.031	1.396
14	-64525521.	-54377500. -54512190. -54447377.	-54970979. -55076192. -55024498.	-54939035. -55063336. -55011093.	1.035	1.379
15	-74072665.	-63199785. -63344096. -63274653.	-63793248. -63908095. -63851770.	-63760755. -63895213. -63838349.	1.039	1.365
16	-84278232.	-72680494. -72834425. -72760352.	-73273942. -73398422. -73337465.	-73240945. -73385516. -73324030.	1.042	1.351
17	-95142223.	-82819626. -82983178. -82904476.	-83413062. -83547173. -83481585.	-83379601. -83534245. -83468137.	1.045	1.339

DIAGONALIZED 1/Z ENERGIES (IN CM-1) FOR THE CARBON1 ISOELECTRONIC SEQUENCE

Z	E0	E1	E2	E2(H.F)	(1S-1D)/(1D-3P) E2	E2(H.F)
18	-106664637.	-93617182.	-94210608.	-94176717.		
		-93780354.	-94354348.	-94341400.		
		-93707023.	-94284129.	-94270668.	1.047	1.328
19	-118845476.	-105873161.	-105666578.	-105632289.		
		-105255955.	-105819947.	-105806979.		
		-105167993.	-105745097.	-105731624.	1.049	1.318
20	-131684737.	-117187564.	-117780972.	-117746314.		
		-117379979.	-117943969.	-117930984.		
		-117287388.	-117864489.	-117851005.	1.051	1.309
21	-145182423.	-129960391.	-130553792.	-130518789.		
		-130162426.	-130726416.	-130713414.		
		-130065206.	-130642305.	-130628810.	1.052	1.300
22	-159338532.	-143391642.	-143985035.	-143949711.		
		-143603298.	-144167286.	-144154269.		
		-143501448.	-144078545.	-144065040.	1.054	1.293
23	-174153065.	-157491316.	-158074703.	-158039078.		
		-157702593.	-158266580.	-158253548.		
		-157596113.	-158173208.	-158159694.	1.055	1.285
24	-189626022.	-172229414.	-172822795.	-172786888.		
		-172460311.	-173024298.	-173011252.		
		-172349202.	-172926296.	-172912773.	1.056	1.278
25	-205757402.	-187635936.	-188229312.	-188193140.		
		-187876454.	-188440439.	-188427381.		
		-187760715.	-188337807.	-188324276.	1.057	1.272
26	-222547206.	-203700881.	-204294252.	-204257830.		
		-203951020.	-204515005.	-204501934.		
		-203833652.	-204407742.	-204394203.	1.058	1.266
27	-239995434.	-220424250.	-221017617.	-220980960.		
		-220684210.	-221247994.	-221234911.		
		-220559012.	-221136101.	-221122555.	1.059	1.260
28	-258102085.	-237806043.	-238399405.	-238362526.		
		-238075423.	-238639407.	-238626313.		
		-237945796.	-238522884.	-238509330.	1.060	1.255
29	-276867161.	-255846260.	-256439618.	-256402528.		
		-256125260.	-256689243.	-256676140.		
		-255991003.	-256568090.	-256554530.	1.060	1.250

DIAGONALIZED 1/Z ENERGIES (IN CM-1) FOR THE CARBON1 ISOELECTRONIC SEQUENCE

Z	E0	E1	E2	E2(H.F)	(1S-1D)/(1D-3P) E2	E2(H.F)
30	-296290659.	-274544900. -274833521. -274694635.	-275138254. -275397503. -275271721.	-275100965. -275384390. -275258154.	1.061	1.245
31	-316372582.	-293901964. -294200205. -294056690.	-294495315. -294764187. -294633775.	-294457837. -294751065. -294620202.	1.062	1.241
32	-337112928.	-313917451. -314225314. -314077168.	-314510799. -314789295. -314654252.	-314473141. -314776162. -314640674.	1.062	1.236
33	-358511698.	-334591362. -334900846. -334756071.	-335184707. -335472826. -335333154.	-335146879. -335459686. -335319570.	1.063	1.232
34	-380568891.	-355923697. -356250801. -356093397.	-356517039. -356814782. -356670479.	-356479048. -356801634. -356656890.	1.063	1.229
35	-403284509.	-377914456. -378251180. -378089146.	-378507795. -378815160. -378666228.	-378469649. -378802005. -378652634.	1.064	1.225
36	-426658549.	-400563638. -400909983. -400743328.	-401156975. -401473963. -401320401.	-401118681. -401460800. -401306801.	1.064	1.222
37	-450691014.	-423871244. -424227210. -424055917.	-424464578. -424791189. -424632997.	-424426143. -424778019. -424619393.	1.065	1.218
38	-475381902.	-447837274. -448202960. -448026938.	-448430606. -448766839. -448604017.	-448392035. -448753662. -448590409.	1.065	1.215
39	-500731214.	-472461727. -472836934. -472656382.	-473055057. -473400913. -473233461.	-473016357. -473387730. -473219848.	1.065	1.212
40	-526738950.	-497744604. -498129432. -497944250.	-498337932. -498693410. -498521329.	-498299107. -498680221. -498507712.	1.066	1.209
41	-553405109.	-523685905. -524080353. -523890542.	-524279231. -524644331. -524467620.	-524240287. -524631136. -524453999.	1.066	1.206

DIAGONALIZED 1/Z ENERGIES (IN CM-1) FOR THE CARBON1 ISCELECTRONIC SEQUENCE

Z	E0	E1	E2	E2(H.F)	(1S-1D)/(1D-3P) E2	E2(H.F)
42	-580729692.	-550285629.	-550878953.	-550839895.		
		-550689699.	-551253676.	-551240475.		
		-550495258.	-551072335.	-551058711.	1.066	1.204
43	-608712699.	-577543777.	-578137130.	-578097932.		
		-577957467.	-578521445.	-578508238.		
		-577758397.	-578335474.	-578321846.	1.067	1.201
44	-637354129.	-605460349.	-606053670.	-606014396.		
		-605883660.	-606447637.	-606434425.		
		-605679960.	-606257036.	-606243405.	1.067	1.199
45	-666653984.	-634035344.	-634628664.	-634589289.		
		-634468276.	-635032253.	-635019036.		
		-634259947.	-634837022.	-634823387.	1.067	1.197
46	-696612261.	-663268763.	-663862081.	-663822609.		
		-663711316.	-664275292.	-664262070.		
		-663498357.	-664075432.	-664061794.	1.068	1.194
47	-727228963.	-693160606.	-693753923.	-693714356.		
		-693612779.	-694176756.	-694163529.		
		-693395191.	-693972266.	-693958624.	1.068	1.192
48	-758504088.	-723710873.	-724304188.	-724264530.		
		-724172667.	-724736643.	-724723411.		
		-723950449.	-724527523.	-724513878.	1.068	1.190
49	-790437637.	-754919563.	-755512877.	-755473131.		
		-755390977.	-755954953.	-755941718.		
		-755164130.	-755741204.	-755727557.	1.068	1.188
50	-823029609.	-786786677.	-787379989.	-787340159.		
		-787267712.	-787831688.	-787818448.		
		-787036235.	-787613309.	-787599658.	1.068	1.186

APPENDIX D

First and second-order spin-orbit corrections for CI.

SPIN-ORBIT INTERACTION

	3P			1D	1S	GROUND ENERGY
	J=0	J=1	J=2	J=2	J=0	
FIRST ORDER	0.0	159.4	462.6	14928.4	28282.6	-81245690.
1S2 2S2 2P 3P	0.0	113.5	332.4	14837.9	28190.7	-81244810.
1S2 2P3 3P	0.0	114.2	333.7	14839.3	28192.1	-81244820.
1S2 2S2 2P 4P	0.0	102.3	299.8	14815.9	28168.4	-81244590.
1S2 2P3 4P	0.0	102.5	300.1	14816.2	28168.8	-81244590.
1S2 2S2 2P 5P	0.0	97.5	285.7	14806.3	28158.8	-81244490.
1S2 2P3 5P	0.0	97.6	285.8	14806.5	28158.9	-81244500.
1S2 2S2 2P 6P	0.0	94.9	278.2	14801.2	28153.6	-81244440.
1S2 2P3 6P	0.0	95.0	278.3	14801.3	28153.7	-81244450.
1S2 2S2 2P 7P	0.0	93.4	273.8	14798.2	28150.6	-81244410.
1S2 2P3 7P	0.0	93.4	273.8	14798.3	28150.6	-81244420.
1S2 2S2 2P 8P	0.0	92.4	270.9	14796.2	28148.6	-81244400.
1S2 2P3 8P	0.0	92.4	270.9	14796.3	28148.6	-81244400.
1S2 2S2 2P 9P	0.0	91.7	268.9	14794.9	28147.2	-81244380.
1S2 2P3 9P	0.0	91.7	268.9	14794.9	28147.2	-81244380.
1S2 2S2 2P 10P	0.0	91.2	267.5	14793.9	28146.2	-81244370.
1S2 2P3 10P	0.0	91.2	267.5	14793.9	28146.3	-81244370.

APPENDIX E

Discrete hydrogenic radial integrals up to, and including, $n = 4$.

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TABLES OF HYDROGENIC SLATER RADIAL INTEGRALS

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Slater radial integrals $R^k(n_1\ell_1 n_2\ell_2;\ n_3\ell_3 n_4\ell_4)$ have been computed as products of powers of primes for hydrogenic radial eigenfunctions for all values of n and ℓ up to $n = 4$ and $\ell = 3$. The decimal equivalents are also tabulated. A number of identities for hydrogenic Slater radial integrals have been discovered.

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CONTENTS

INTRODUCTION

Over the past few years there has been a considerable interest in the reinterpretation of the properties of the hydrogen atom in terms of the conformal group O(4,2).[1,2] Cunningham[3,4] has used the O(3) × O(2,1) subgroup of O(4,2) to study the properties of the hydrogen radial matrix elements of r^k making use of the fact that the hydrogen radial eigenfunctions span infinite dimension representations of the noncompact group O(2,1). Similar work has been undertaken by Armstrong[5] and Feneuille.[6] This work has largely explained the radial-matrix-element selection rules found earlier by Pasternack and Sternheimer.[7]

So far no attempt has been made to extend the group theoretical analyses to the Slater radial integrals that arise in the calculation of the two-particle Coulomb-repulsion matrix elements associated with many-electron atoms. There is good reason to believe that such analyses should first be directed towards understanding the properties of Slater radial integrals in which hydrogenic eigenfunctions are used. Hydrogenic Slater radial integrals can also play an important role in the development of perturbative calculations of many-electron atoms[8,9] and in the study of R_4 models of atomic energy levels.[10]

Studies such as the above are severely hampered by the lack of any detailed tables of hydrogenic radial integrals. If one is looking for systematics among these integrals it is highly desirable to have tables calculated in terms of powers of prime numbers.

In this paper we present a table of hydrogenic Slater radial integrals in terms of powers of primes and as decimal equivalents. The values were calculated from a program written for an IBM 360/44 computer.

CALCULATION OF RADIAL INTEGRALS

The normalized nonrelativistic hydrogen wavefunctions can be written as[11]

$$\psi_{n\ell m}(r,\theta,\varphi) = a^{-3/2}\, N_{n\ell}\, R_{n\ell}\left(\frac{2r}{na}\right) Y_\ell^m\,(\theta,\varphi)$$

with

$$N_{n\ell} = \frac{2}{n^2}\left[\frac{(n-\ell-1)!}{[(n+\ell)!]^3}\right]^{1/2}$$

and

$$R_{n\ell}(x) = x^\ell\, e^{-x/2}\, L_{n-\ell-1}^{2\ell+1}(x). \tag{1}$$

Here $a = \hbar^2/Zme^2$, the $Y_\ell^m(\theta,\varphi)$ are the usual normalized spherical harmonics, and the $L_b^a(z)$ the usual Laguerre polynomials.

The matrix elements of the Coulomb repulsion $\sum_{i<j} e^2/r_{ij}$ may be factorized into the product of an angular matrix element and a radial matrix element. The latter matrix element is normally designated the Slater radial integral and may be written in atomic units as[12]

$$R^k(ab,cd) = \int_0^\infty \int_0^\infty \frac{r_<^k}{r_>^{k+1}} R_a(r_1)R_b(r_2)R_c(r_1)R_d(r_2) r_1^2 r_2^2 dr_1 dr_2 \tag{2}$$

where $r_<$ is the lesser and $r_>$ the greater of r_1 and r_2. Eq. (2) may in turn be written in terms of a linear combination of integrals of the form

$$\int_0^\infty r_1^p e^{-\alpha r_1} \int_0^r r_2^q e^{-\beta r_2}\, dr_2 dr_1 = \frac{p!q!}{\alpha^{p+1}\beta^{q+1}} - \sum_{s=0}^{q} \frac{1}{\beta^{s+1}} \frac{(p+q-s)!}{(\alpha+\beta)^{p+q+1-s}}$$

to yield finally the result

$$R^k(ab,cd) = A(abcd) \sum_{s=0}^{n_a-\ell_a-1} \sum_{s_1=0}^{\cdots} \sum_{s_2=0}^{\cdots} \sum_{s_3=0}^{n_d-\ell_d-1} A(s)B(s_1) \times C(s_2)D(s_3)I(s\, s_1\, s_2\, s_3)$$

where

$$A(abcd) = \frac{2^4}{(n_a n_b n_c n_d)^2}[(n_a-\ell_a-1)!\ldots(n_d-\ell_d-1)!]^{1/2} \times \left(\frac{2}{n_a}\right)^{\ell_a} \cdots \left(\frac{2}{n_d}\right)^{\ell_d}$$

and

$$A(s) = \frac{(-1)^s \left(\frac{2}{n_a}\right)^s}{(n_a - \ell_a - 1 - s)!(2\ell_a + 1 + s)!s!}$$

with similar expressions for $B(s_1)$, $C(s_2)$, and $D(s_3)$. Finally,

$$I(s\, s_1\, s_2\, s_3) = \frac{q!}{\alpha^{q+1}\beta^{p+1}} \left(\frac{\beta}{\alpha+\beta}\right)^{p+1} \sum_{r=0}^{q} \frac{(p+r)!}{r!} \left(\frac{\alpha}{\alpha+\beta}\right)^r + \frac{y!}{\alpha^{x+1}\beta^{y+1}} \left(\frac{\alpha}{\alpha+\beta}\right)^{x+1} \sum_{r=0}^{y} \frac{(x+r)!}{r!} \left(\frac{\beta}{\alpha+\beta}\right)^r$$

where

$$\begin{aligned} p &= \ell_b + \ell_d + 2 + k + s_1 + s_3 \\ q &= \ell_a + \ell_c + 1 - k + s + s_2 \\ x &= \ell_a + \ell_c + 2 + k + s + s_2 \\ y &= \ell_b + \ell_d + 1 - k + s_1 + s_3 \\ \alpha &= (n_a + n_c)/n_a n_c \\ \beta &= (n_b + n_d)/n_b n_d. \end{aligned}$$

The above results were used to construct a computer program for evaluating the hydrogenic Slater radial integrals. All of the arithmetic operations were done by a powers-of-prime-numbers routine. The largest integer used in the IBM 360/44 with the normal register operations is of the order of 10^9. Since some additions gave rise to integers in excess of this value, it was necessary for one of us (P.H.B.) to develop a multiple precision powers-of-primes program to overcome this difficulty. A few of the final results had to be converted from the machine form into prime form by hand as did their associated decimal values. Such integrals always involved a very large last factor.

SOME IDENTITIES

There are a number of equalities between the integrals. They are

$$\begin{aligned} R0(2s2s,2s1s) &= R0(2p2s,2p1s) \\ R0(3p3p,3p2p) &= R0(3d3p,3d2p) \\ R0(4d4d,4d3d) &= R0(4f4d,4f3d) \\ R1(2p2p,2s2s) &= R2(2p2p,2p2p) \\ R2(4f2p,4p2p) &= -R1(4f2p,4d2s) \\ R0(4d4d,4d4d) &= R0(4f4p,4f4p). \\ R3(5g5g,5p5p) &= R6(5g5g,5d5d) \end{aligned}$$

The first three equalities satisfy the relation

$$R0(nn - 2\,nn - 2, nn - 2\,n - 1n - 2) = R0(nn - 1\,nn - 2, nn - 1\,n - 1n - 2).$$

The rule has been verified by calculation up to $n = 9$. No such relation involving the remaining cases has been found. At present we are investigating these equalities by means of the O(2.1) algebra.

Acknowledgment

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TABLES OF HYDROGENIC SLATER RADIAL INTEGRALS

Explanation of Tables

Tabulated are values of $R^k(ab,cd)$ (Eq. 2) in both decimal and power-of-prime notation.
The radial integral $R^k(ab,cd)$ has the following permutational symmetries

$$R^k(ab,cd) \equiv R^k(cb,ad) \equiv R^k(ad,cb) \equiv R^k(ba,dc).$$

The table is arranged with the largest principal quantum number in the left-most position and the next largest in the second position, when possible, etc. This order was strictly followed, and a similar ordering was used in the angular quantum numbers where possible. For a given set of quantum numbers all the parity-allowed k-values are tabulated.

The decimal form carries with it the overall sign of the radial integral. Twice the powers of the first six primes are listed, followed by the higher prime factors set between periods (full stops). This latter part is factorized into primes up to 1000, so any factor greater than 10^6 need not be a prime. The notation .31*2. is to be interpreted as 31^2, etc.

As an example we have from the table

R0(3s1s,2s1s) 0.0505265 25 7 −10, 0 2 0 .17* −6.1279.

which is to be read as

$$\begin{aligned} \text{R0(3s1s,2s1s)} &= (2^{25} \times 3^7 \times 5^{-10} \times 11^2)^{1/2} \times 17^{-6} \times 1279 \\ &= 0.0505265 \text{ (atomic units).} \end{aligned}$$

For a negative integral we have as an example

R1(3p2p,2s1s) −0.0045861 11 2 −8, −14 0 0 .17387.

giving us

$$\begin{aligned} \text{R1(3p2p,2s1s)} &= -(2^{11} \times 3^2 \times 5^{-8} \times 7^{-14})^{1/2} \times 17387 \\ &= -0.0045861. \end{aligned}$$

The tables are calculated for nuclear charge one, for other values just multiply by Z.

TABLES OF HYDROGENIC SLATER RADIAL INTEGRALS

INTEGRAL	VALUE	2× (POWER OF FIRST SIX PRIMES)						ADDITIONAL FACTORS
R0(1S1S,1S1S)	0.6250000	-6	0	2,	0	0	0	
R0(2S1S,1S1S)	0.0893550	25	-6	0,	-8	0	0	
R0(2S1S,2S1S)	0.2098765	0	-8	0,	0	0	0	.17.
R0(2P1S,2P1S)	0.2427984	0	-10	0,	0	0	0	.59.
R0(2S2S,1S1S)	0.0219479	8	-12	0,	0	0	0	
R1(2P2P,1S1S)	0.0512117	8	-14	0,	2	0	0	
R0(2S2S,2S1S)	0.0085817	19	-6	-10,	0	0	0	
R0(2P2S,2P1S)	0.0085817	19	-6	-10,	0	0	0	
R1(2P2P,2S1S)	-0.0386175	17	-2	-10,	0	0	0	
R0(2S2S,2S2S)	0.1503906	-18	0	0,	2	2	0	
R0(2P2S,2P2S)	0.1621094	-18	0	0,	0	0	0	.83.
R1(2P2P,2S2S)	0.0878906	-18	4	2,	0	0	0	
R0(2P2P,2P2P)	0.1816406	-18	2	0,	0	0	0	.31.
R2(2P2P,2P2P)	0.0878906	-18	4	2,	0	0	0	
R0(3S1S,1S1S)	0.0439594	-8	7	-10,	0	0	0	.47.
R0(3S1S,2S1S)	0.0505265	25	7	-10,	0	2	0	.17*-6.1279.
R0(3P1S,2P1S)	0.0573912	30	8	-10,	2	0	0	.17*-6.233.
R0(3S1S,3S1S)	0.0994873	-26	0	2,	0	0	0	.163.
R0(3P1S,3P1S)	0.1088257	-28	0	0,	0	0	0	.1783.
R0(3D1S,3D1S)	0.1110229	-28	0	0,	0	0	0	.17.107.
R0(3S2S,1S1S)	0.0112229	25	7	0,	0	0	0	.17*-6.
R1(3P2P,1S1S)	0.0262535	10	2	0,	2	0	0	.17*-6.23.41.
R0(3S2S,1S2S)	0.0039360	-8	7	0,	-14	0	0	.1109.
R0(3S2P,1S2P)	0.0034817	-8	11	0,	-14	0	0	.109.
R1(3P2P,1S2S)	-0.0170566	-5	12	0,	-14	0	0	.109.
R2(3D2P,1S2P)	0.0097867	-1	7	1,	-14	0	0	.109.
R0(3S2S,2S1S)	0.0045428	8	7	2,	-14	0	0	
R1(3S2P,2P1S)	-0.0136699	8	3	-8,	-14	0	0	.84631.
R0(3P2S,2P1S)	0.0044511	11	8	0,	-14	0	0	
R1(3P2P,2S1S)	-0.0045861	11	2	-8,	-14	0	0	.17387.
R1(3D2P,2P1S)	0.0239252	11	3	-9,	-14	0	0	.117101.
R0(3S2S,2S2S)	0.0214671	19	7	-10,	0	-16	0	.331.1283.
R0(3S2P,2S2P)	0.0265220	19	11	-10,	0	-16	0	.97.601.
R1(3S2P,2P2S)	0.0210219	17	13	-8,	0	-16	0	.61.101.
R0(3P2S,2P2S)	0.0209143	24	8	-10,	0	-16	0	.42227.
R1(3P2P,2S2S)	-0.0009918	22	12	-8,	0	-16	0	.89.
R0(3P2P,2P2P)	0.0286531	28	12	-10,	0	-16	0	.1607.
R2(3P2P,2P2P)	0.0179385	20	8	-4,	0	-16	0	.19.61.
R2(3D2P,2S2P)	-0.0456697	24	7	-5,	0	-16	0	.2857.
R1(3D2P,2P2S)	-0.0554865	26	13	-9,	0	-16	0	.1607.
R0(3S2S,3S1S)	0.0024289	25	-6	2,	0	0	-16	.1847.
R0(3P2S,3P1S)	0.0023649	35	-6	0,	0	0	-16	.281.
R1(3P2P,3S1S)	-0.0119788	28	-1	0,	0	0	-16	.1033.
R0(3D2S,3D1S)	0.0003198	37	-6	0,	0	0	-16	.19.
R1(3D2P,3P1S)	-0.0027869	33	-1	1,	0	0	-16	.19.
R0(3S2S,3S2S)	0.0841139	0	0	-16,	0	2	0	.29.103.
R0(3S2P,3S2P)	0.0867558	0	0	-16,	0	0	0	.33889.
R0(3P2S,3P2S)	0.0000122	0	0	-16,	2	0	0	.5023.
R1(3P2P,3S2S)	0.0352162	9	7	-16,	0	0	2	
R0(3P2P,3P2P)	0.0939443	0	0	-16,	0	0	0	.36697.
R2(3P2P,3P2P)	0.0258816	2	2	-14,	0	0	0	.337.
R0(3D2S,3D2S)	0.1035781	0	0	-18,	0	2	0	.53.347.
R2(3D2P,3S2P)	0.0015543	13	2	-15,	0	0	0	
R1(3D2P,3P2S)	0.0239869	12	7	-17,	2	0	0	
R0(3D2P,3D2P)	0.1063306	0	0	-18,	0	0	0	.97.2141.
R2(3D2P,3D2P)	0.0371251	2	2	-16,	0	0	0	.2417.

INTEGRAL	VALUE	2× (POWER OF FIRST SIX PRIMES)	ADDITIONAL FACTORS
R0(3S3S,1S1S)	0.0057678	-30 6 0, 2 0 0	
R1(3P3P,1S1S)	0.0135956	-32 8 0, 0 2 0	
R2(3D3D,1S1S)	0.0012360	-32 8 0, 0 0 0	
R0(3S3S,2S1S)	0.0021090	25 6 0, 0 2-16	
R1(3S3P,2P1S)	-0.0063486	10 11 -8, 0 0-16	.240319.
R0(3P3S,2P1S)	0.0018786	30 7 0, 0 0-16	
R1(3P3P,2S1S)	-0.0023283	15 8 -8, 0 0-16	.73.1109.
R2(3P3D,2P1S)	0.0028544	23 7 -5, 0 0-16	.31*2.
R1(3D3P,2P1S)	0.0106504	17 11 -9, 2 0-16	.11383.
R2(3D3D,2S1S)	-0.0039205	29 10 -6, 0 0-16	.71.
R0(3S3S,2S2S)	0.0074760	8 6-20, 0 0 4	
R1(3S3S,2P2P)	0.0094224	8 8-20, 0 0 0	.71.
R1(3P3S,2S2P)	0.0058513	11 13-20, 0 0 0	
R0(3P3S,2P2S)	0.0080185	11 7-20, 0 0 0	.37.
R1(3P3P,2S2S)	0.0084935	20 8-20, 0 0 0	
R0(3P3P,2P2P)	0.0099090	18 6-20, 2 0 0	
R2(3P3P,2P2P)	0.0113246	24 6-20, 0 0 0	
R1(3D3S,2P2P)	-0.0102399	11 8-21, 0 0 0	.61.
R2(3D3P,2S2P)	0.0005483	16 7-21, 0 0 0	
R1(3D3P,2P2S)	0.0049343	16 11-21, 0 0 0	
R2(3D3D,2S2S)	0.0365219	18 8-22, 0 0 0	.43.
R1(3D3D,2P2P)	0.0373712	22 8-22, 0 2 0	
R3(3D3D,2P2P)	0.0217999	18 6-22, 2 2 0	
R0(3S3S,3S1S)	0.0011311	-8-19 0, 0 0 0	.617.
R0(3P3S,3P1S)	0.0010138	-8-19 0, 2 0 0	.79.
R1(3P3P,3S1S)	-0.0051258	-4-17 0, 0 0 0	.233.
R2(3P3D,3P1S)	0.0024117	3-19 1, 0 0 2	
R0(3D3S,3D1S)	0.0000752	-8-19 0, 0 0 0	.41.
R1(3D3P,3P1S)	-0.0007131	-7-17 1, 0 0 0	.41.
R2(3D3D,3S1S)	-0.0003667	-2-19 4, 0 0 0	
R2(3D3D,3D1S)	0.0028476	-1-19 -1, 0 0 0	.307.
R0(3S3S,3S2S)	0.0046473	25-37-10, 2 0 0	.149.1613.
R0(3S3P,3S2P)	0.0046104	30-36-10, 0 0 0	.170341.
R1(3P3S,3S2P)	0.0001975	28-34 -8, 2 0 0	.139.
R0(3P3S,3P2S)	0.0055192	35-37-10, 0 0 0	.29.2153.
R1(3P3P,3S2S)	-0.0117856	33-35 -8, 0 0 0	.29.613.
R0(3P3P,3P2P)	0.0058791	44-36-10, 0 0 0	.1697.
R2(3P3P,3P2P)	-0.0041808	26-36 -4, 0 0 0	.4943.
R1(3P3D,3S2P)	-0.0278869	43-34 -9, 0 0 0	.1697.
R2(3P3D,3P2S)	-0.0247089	32-37 -5, 0 0 0	.14143.
R1(3D3S,3P2P)	-0.0043573	33-34 -7, 0 0 0	.1697.
R0(3D3S,3D2S)	0.0069004	37-37-10, 0 0 0	.23.1697.
R2(3D3P,3S2P)	-0.0090724	39-36 -3, 0 0 0	.53.
R1(3D3P,3P2S)	-0.0142310	38-35 -7, 0 0 0	.1697.
R0(3D3P,3D2P)	0.0058791	44-36-10, 0 0 0	.1697.
R2(3D3P,3D2P)	-0.0065741	26-36 -6, 0 2 0	.3533.
R2(3D3D,3S2S)	-0.0121102	41-37 -4, 0 0 0	.137.
R1(3D3D,3P2P)	-0.0220465	40-34 -8, 0 0 0	.1697.
R3(3D3D,3P2P)	-0.0108939	34-36 -2, 2 0 0	.23.
R2(3D3D,3D2S)	-0.0370600	32-37 -7, 0 0 0	.17*2.367.
R0(3S3S,3S3S)	0.0664062	-16 0 0, 0 0 0	.17.
R0(3P3S,3P3S)	0.0687934	-18 -4 0, 0 0 0	.317.
R1(3P3P,3S3S)	0.0423177	-18 -2 2, 0 0 2	
R0(3P3P,3P3P)	0.0718678	-20 -6 0, 0 0 0	.1987.
R2(3P3P,3P3P)	0.0359881	-20 -6 2, 0 0 0	.199.
R0(3D3S,3D3S)	0.0731337	-18 -4 0, 0 0 0	.337.
R2(3D3P,3S3P)	0.0257347	-19 -2 5, 0 0 0	
R1(3D3P,3P3S)	0.0360286	-19 -2 3, 2 0 0	
R0(3D3P,3D3P)	0.0769314	-20 -4 0, 0 0 0	.709.
R2(3D3P,3D3P)	0.0361328	-20 0 0, 0 0 0	.37.
R2(3D3D,3S3S)	0.0227865	-18 -2 2, 2 0 0	
R1(3D3D,3P3P)	0.0341797	-20 0 2, 2 0 0	
R3(3D3D,3P3P)	0.0240524	-20 -6 2, 2 0 0	.19.
R2(3D3D,3D3S)	0.0243622	-19 -4 1, 0 0 0	.71.
R0(3D3D,3D3D)	0.0860460	-20 -4 0, 0 0 2	.61.
R2(3D3D,3D3D)	0.0454210	-20 -4 -2, 2 0 2	.23.

INTEGRAL	VALUE	2× (POWER OF FIRST SIX PRIMES)	ADDITIONAL FACTORS
R4(3D3D,3D3D)	0.0296224	-20 -2 0, 2 0 2	
R0(4S1S,1S1S)	0.0276069	34 4-10, 0 0-12	.353.
R0(4S1S,2S1S)	0.0287157	31-12 0, 0-14 0	.8803.
R0(4P1S,2P1S)	0.0320504	33-12 1, 0-14 6	
R0(4S1S,3S1S)	0.0288387	34 7 2,-14 0 0	.19.31*-8.34785431.
R0(4P1S,3P1S)	0.0324144	41 8 1,-14 0 0	.31*-8.191.347.1279.
R0(4D1S,3D1S)	0.0273452	45 11 0,-14 2 0	.31*-8.699401.
R0(4S1S,4S1S)	0.0576333	0 0-16, 0 0 0	.47.479.
R0(4P1S,4P1S)	0.0615163	0 0-18, 0 0 0	.137.877.
R0(4D1S,4D1S)	0.0624502	0 0-18, 0 0 0	.283.431.
R0(4F1S,4F1S)	0.0624993	0 0-18, 0 0 0	.122069.
R0(4S2S,1S1S)	0.0071341	31 2 0, 0-14 0	
R1(4P2P,1S1S)	0.0166847	25 -2 -9, 0-14 0	.17.109.127.
R0(4S2S,1S2S)	0.0024273	28-30-10, 2 0 2	.73.
R0(4S2P,1S2P)	0.0020466	32-32-10, 0 0 0	.4201.
R1(4P2P,1S2S)	-0.0102970	28-28 -9, 0 0 0	.4201.
R2(4D2P,1S2P)	0.0070434	26-32 -5, 0 0 0	.2069.
R0(4S2S,2S1S)	0.0029180	28-34 0, 0 0 0	.23.
R1(4S2P,2P1S)	-0.0080245	24-34 0, 0 2 0	.23.
R0(4P2S,2P1S)	0.0028369	30-34 3, 0 0 0	
R1(4P2P,2S1S)	-0.0013830	22-32 1, 0 0 2	
R1(4D2P,2P1S)	0.0151774	26-34 1, 0 0 0	.107.
R0(4S2S,2S2S)	0.0105541	25-12 0,-16 0 2	.19.31.
R0(4S2P,2S2P)	0.0135686	29-12 0,-16 0 0	.23.107.
R1(4S2P,2P2S)	0.0108918	27 -8 0,-16 0 0	.439.
R0(4P2S,2P2S)	0.0098073	27-12 1,-16 0 0	.37.43.
R1(4P2P,2S2S)	-0.0039112	25 -6 1,-16 0 0	.47.
R0(4P2P,2P2P)	0.0143010	35-12 3,-16 0 0	.29.
R2(4P2P,2P2P)	0.0082801	23 -6 1,-16 0 0	.199.
R2(4D2P,2S2P)	-0.0266710	23 -6 1,-16 0 0	.641.
R1(4D2P,2P2S)	-0.0321772	31 -8 3,-16 0 0	.29.
R2(4F2P,2P2P)	0.0110228	25 -7 1,-17 0 0	.607.
R0(4S2S,3S1S)	0.0015651	31 7-34, 0 0 0	.19.29.
R1(4S2P,3P1S)	-0.0057306	32 2-34,-12 0 0	.73.35839087.
R0(4P2S,3P1S)	0.0015185	38 8-35, 0 0 0	.61.
R1(4P2P,3S1S)	-0.0039039	25 3-35,-12 0 2	.31.64594697.
R1(4P2P,3D1S)	-0.0007580	36 3-36,-12 0 0	.249750119.
R0(4D2S,3D1S)	0.0002314	42 11-36, 0 0 0	
R1(4D2P,3P1S)	0.0036617	34 6-35,-12 0 0	.61.593.5741.
R1(4F2P,3D1S)	0.0076781	40 6-36,-13 2 0	.997.29363.
R0(4S2S,3S2S)	0.0190414	28 7 0,-14 0 2	.19*-10.37.41.131.48571.
R0(4S2P,3S2P)	0.0206947	32 11 0,-14 0 0	.19*-10.31.151.809273.
R1(4S2P,3P2S)	0.0143361	35 12 0,-12 0 0	.19*-10.76524661.
R2(4S2P,3D2P)	0.0009392	39 7 1,-10 0 0	.19*-10.383.3259.
R0(4P2S,3P2S)	0.0205746	35 8 1,-14 0 0	.19*-10.31.99815293.
R1(4P2P,3S2S)	0.0085607	28 13 1,-12 0 0	.19*-10.761.175411.
R0(4P2P,3P2P)	0.0230004	43 12 1,-14 0 0	.19*-10.24021553.
R2(4P2P,3P2P)	0.0120623	31 8 1,-10 0 0	.19*-10.148089121.
R1(4P2P,3D2S)	0.0098368	49 13 0,-12 0 0	.19*-10.163.1453.
R0(4D2S,3D2S)	0.0223860	39 11 0,-14 0 0	.19*-10.362199283.
R2(4D2P,3S2P)	-0.0076810	26 11 1,-10 0 0	.19*-10.102660139.
R1(4D2P,3P2S)	-0.0049508	39 16 1,-12 0 0	.19*-10.328291.
R0(4D2P,3D2P)	0.0241675	45 19 0,-14 0 0	.19*-10.603431.
R2(4D2P,3D2P)	0.0162521	37 11 0,-10 0 0	.19*-10.10732847.
R2(4F2P,3P2P)	-0.0102566	33 11 1,-11 0 0	.19*-10.32057603.
R1(4F2P,3D2S)	-0.0276874	41 20 0,-13 0 0	.19*-10.603431.
R0(4S2S,4S1S)	0.0010096	-35 -6 0, 0 0 0	.31.163.
R0(4P2S,4P1S)	0.0009773	-35 -6 0, 0 0 0	.67.73.
R1(4P2P,4S1S)	-0.0051188	-35 -2 1, 0 0 0	.19.67.
R0(4D2S,4D1S)	0.0001680	-35 -6 0, 0 0 0	.29*2.
R1(4D2P,4P1S)	-0.0013253	-35 -2 0, 0 2 0	.67.
R0(4F2S,4F1S)	0.0000062	-35 -6 0, 0 0 0	.31.
R1(4F2P,4S1S)	0.0000623	-35 -3 1, -1 0 0	.71.
R1(4F2P,4D1S)	-0.0000852	-35 -3 0, 1 0 0	.31.

INTEGRAL	VALUE	2× (POWER OF FIRST SIX PRIMES)	ADDITIONAL FACTORS
R0(4S2S,4S2S)	0.0513514	-4-18 0, 0 0 0 2	.311.
R0(4S2P,4S2P)	0.0524014	-4-20 0, 0 0 0 0	.12377.
R0(4P2S,4P2S)	0.0539933	-4-16 0, 0 0 0 2	.109.
R1(4P2P,4S2S)	0.0156774	2-16 1, 0 0 0 0	.23.
R0(4P2P,4P2P)	0.0555175	-4-16 0, 0 0 0 0	.31.47.
R2(4P2P,4P2P)	0.0099070	0-16 2, 0 0 0 2	
R0(4D2S,4D2S)	0.0590738	-4-18 0, 0 0 0 0	.4651.
R2(4D2P,4S2P)	-0.0003787	2-20 3, 0 0 0 0	
R1(4D2P,4P2S)	0.0106691	2-16 2, 2 0 0 0	
R0(4D2P,4D2P)	0.0602593	-4-20 0, 0 0 0 0	.43.331.
R2(4D2P,4D2P)	0.0130908	0-20 0, 0 0 0 0	.773.
R0(4F2S,4F2S)	0.0621221	-4-18 0, 0 0 0 0	.67.73.
R1(4F2P,4S2S)	-0.0010412	2-17 1, 1 0 0 0	
R2(4F2P,4P2P)	-0.0023282	2-17 2, 1 0 0 0	
R1(4F2P,4D2S)	0.0023282	2-17 2, 1 0 0 0	
R0(4F2P,4F2P)	0.0622915	-4-20 0, 0 0 0 0	.14713.
R2(4F2P,4F2P)	0.0098828	0-20 2, -2 0 0 0	.19.43.
R0(4S3S,1S1S)	0.0036725	34 7 0, 2 0 0 0	.31*-8.73.
R1(4P3P,1S1S)	0.0086683	17 12 -9, 0 0 0 0	.31*-8.39148147.
R2(4D3D,1S1S)	0.0009020	29 7 -6, 0 0 0 2	.31*-8.6827.
R0(4S3S,1S2S)	0.0013033	31 7-38, 0 0 0 0	.11471.
R0(4S3P,1S2P)	0.0011177	40 8-38, 0 0 0 0	.251.
R1(4P3S,1S2P)	-0.0038883	25 13-39, 2 0 0 0	.41.79.
R1(4P3P,1S2S)	-0.0014523	30 12-39, 0 0 0 0	.2593.
R1(4P3D,1S2P)	0.0064617	32 13-40, 0 2 0 0	.677.
R2(4D3P,1S2P)	0.0021259	38 8-37, 2 0 0 0	.61.
R2(4D3D,1S2S)	-0.0027239	38 7-38, 0 0 0 2	.163.
R3(4F3D,1S2P)	0.0004736	40 10-40, 1 0 0 0	.67.
R0(4S3S,1S3S)	0.0006997	34 2-10, 2 0 0 0	.23*-10.32908807.
R0(4S3P,1S3P)	0.0006072	48 2-10, 0 0 0 0	.23*-10.1561883.
R0(4S3D,1S3D)	0.0000350	54 2-10, 0 0 0 0	.23*-10.11251.
R1(4P3P,1S3S)	-0.0030758	39 7 -9, 0 0 0 2	.23*-10.179.2207.
R1(4P3D,1S3P)	-0.0003409	48 7 -8, 0 0 0 0	.23*-10.11251.
R2(4D3P,1S3P)	0.0017008	32 2 -5, 0 0 0 0	.23*-10.20033309.
R2(4D3D,1S3S)	-0.0003052	45 2 -4, 0 0 0 0	.23*-10.17761.
R2(4D3D,1S3D)	0.0019443	32 2 -7, 0 0 0 0	.23*-10.97.1180477.
R3(4F3D,1S3P)	-0.0000471	38 4 -2, 1 2 0 0	.23*-10.71.
R0(4S3S,2S1S)	0.0013606	31 7-34, 0 0 0 0	.479.
R1(4S3P,2P1S)	-0.0037786	16 -4-34, 0 0 0 0	.17.5961731.
R0(4P3S,2P1S)	0.0012119	33 11-35, 0 0 0 0	.53.
R1(4P3P,2S1S)	-0.0007997	14 -2-35, 0 0 0 0	.73.127.3449.
R2(4P3D,2P1S)	0.0015224	26 1-34, 0 0 0 0	.23.3559.
R1(4D3P,2P1S)	0.0068497	18 -4-35, 0 0 0 2	.479.32987.
R2(4D3D,2S1S)	-0.0024055	26 1-34, 0 0 0 0	.211.613.
R2(4F3D,2P1S)	0.0008867	28 0-34, -1 2 0 0	.9931.
R0(4S3S,2S2S)	0.0041639	28 7 0, 0 2 2	.19*-10.233.
R1(4S3S,2P2P)	0.0054455	24 -3 -8, 0 0 0	.19*-10.26471372569.
R0(4S3P,2S2P)	0.0046187	37 8 0, 0 0 0	.19*-10.23.41.
R1(4S3P,2P2S)	0.0038114	29 -4 -8, 0 0 2	.19*-10.436384813.
R1(4S3D,2P2P)	-0.0049192	31 -3 -9, 0 0 0	.19*-10.47.83.1211531.
R1(4P3S,2S2P)	0.0024355	22 -1 -7, 0 0 0	.19*-10.29.121715261.
R0(4P3S,2P2S)	0.0042503	30 11 3, 0 0 4	.19*-10.
R1(4P3P,2S2S)	0.0047508	27 -2 -7, 2 0 0	.19*-10.301170367.
R0(4P3P,2P2P)	0.0055198	43 12 1, 2 0 0	.19*-10.
R2(4P3P,2P2P)	0.0065660	35 2 -5, 0 0 0	.19*-10.4046851.
R1(4P3D,2S2P)	0.0048785	29 -1 -8, 0 0 0	.19*-10.43.89.365147.
R2(4P3D,2P2S)	0.0020619	35 1 -6, 0 0 0	.19*-10.4921883.
R1(4D3S,2P2P)	-0.0073056	26 -3 -7, 0 0 0	.19*-10.7941072431.
R2(4D3P,2S2P)	-0.0016418	35 2 -5, 4 0 0	.19*-10.107.193.
R1(4D3P,2P2S)	0.0009789	31 -4 -7, 0 0 0	.19*-10.325787569.
R2(4D3D,2S2S)	0.0139562	35 1 -6, 0 0 0	.19*-10.79.572777.
R1(4D3D,2P2P)	0.0207566	33 -3 -8, 0 0 0	.19*-10.101.163.439.617.
R3(4D3D,2P2P)	0.0123165	47 3 4, 4 0 0	.19*-10.
R2(4F3P,2P2P)	-0.0011970	37 1 -5, -1 0 0	.19*-10.197.8581.
R3(4F3D,2S2P)	-0.0082033	37 4 -2, 1 0 0	.19*-10.61.467.
R2(4F3D,2P2S)	-0.0100999	37 0 -6, -1 0 0	.19*-10.43.53.24239.

INTEGRAL	VALUE	2× (POWER OF FIRST SIX PRIMES)	ADDITIONAL FACTORS
R0(4S3S,2S3S)	0.0020743	31-12 0, 0 0 0	.17*-11.41.27276299.
R0(4S3P,2S3P)	0.0024407	45-12 0, 0 0 0	.17*-11.10280261.
R1(4S3P,2P3S)	-0.0001119	38 -7 0, 0 0 0	.17*-11.341963.
R0(4S3D,2S3D)	0.0026946	51-12 0, 0 0 0	.17*-11.107.13259.
R1(4S3D,2P3P)	-0.0030560	47 -7 1, 0 0 0	.17*-11.29.6367.
R0(4P3S,2P3S)	0.0020558	33-12 1, 0 0 0	.17*-11.247836469.
R1(4P3P,2S3S)	-0.0065069	36 -5 1, 2 0 0	.17*-11.797.1063.
R0(4P3P,2P3P)	0.0026816	51-12 1, 0 0 0	.17*-11.631409.
R2(4P3P,2P3P)	-0.0021691	29 -4 1, 0 0 0	.17*-11.53.167.1459.
R1(4P3D,2S3P)	-0.0079840	45 -5 2, 0 0 4	.17*-11.23.37.
R2(4P3D,2P3S)	-0.0046613	46 -4 2, 2 0 0	.17*-11.59.83.
R0(4P3D,2P3D)	0.0020964	55-12 1, 0 0 0	.17*-11.12347.
R2(4P3D,2P3D)	-0.0048448	29 -4 -1, 0 0 0	.17*-11.157.593.1549.
R2(4D3P,2S3P)	-0.0095926	29 -4 1, 0 0 0	.17*-11.31.1842199.
R1(4D3P,2P3S)	-0.0127636	42 -7 1, 0 0 0	.17*-11.4362367.
R2(4D3D,2S3S)	-0.0026657	42 -4 4, 0 0 0	.17*-11.15683.
R2(4D3D,2S3D)	-0.0168803	29 -4 -1, 0 2 0	.17*-11.45679099.
R1(4D3D,2P3P)	-0.0091344	49 -7 2, 0 0 0	.17*-11.123407.
R3(4D3D,2P3P)	-0.0033948	55 -3 2, 4 0 2	.17*-11.
R2(4F3P,2P3P)	0.0085401	31 -5 1, -1 0 0	.17*-11.37.3148499.
R3(4F3D,2S3P)	0.0080812	35 -2 2, 1 0 0	.17*-11.59.5743.
R2(4F3D,2P3S)	0.0052796	44 -5 2, -1 0 0	.17*-11.355847.
R2(4F3D,2P3D)	0.0115116	31 -5 -1, 1 0 0	.17*-11.112162249.
R4(4F3D,2P3D)	0.0074780	43 5 1, 1 0 0	.17*-11.937.
R0(4S3S,3S1S)	0.0007303	34 6 0, 0 0 0	.23*-10.83.103.
R1(4S3P,3P1S)	-0.0025181	24 8 0,-12 0 0	.23*-10.73.506715113.
R2(4S3D,3D1S)	-0.0002005	42 8 0,-10 0 0	.23*-10.59.13931.
R0(4P3S,3P1S)	0.0006551	41 7 5, 2 0 0	.23*-10.
R1(4P3P,3S1S)	-0.0017446	17 11 3,-12 0 0	.17.23*-10.71.4135073.
R1(4P3P,3D1S)	-0.0000745	28 11 0,-12 0 0	.23*-10.52645031.
R2(4P3D,3P1S)	0.0012598	34 7 0,-10 0 0	.23*-10.631.226789.
R0(4D3S,3D1S)	0.0000580	45 8 2, 0 0 0	.23*-10.
R1(4D3P,3P1S)	0.0017678	26 10 1,-12 0 0	.23*-10.1935646241.
R2(4D3D,3S1S)	-0.0007796	29 8 0,-10 0 0	.23*-10.289199483.
R2(4D3D,3D1S)	0.0013938	40 8 -1,-10 0 0	.19.23*-10.631.2131.
R1(4F3P,3D1S)	0.0031345	32 10 0,-13 0 0	.23*-10.2538009121.
R2(4F3D,3P1S)	-0.0005738	36 8 0,-11 0 0	.23*-10.109.456679.
R0(4S3S,3S2S)	0.0028538	31 6 0, 2 0 2	.17*-11.859.
R1(4S3S,3P2P)	0.0017230	32 11 -8,-12 0 0	.17*-11.239.658639171.
R0(4S3P,3S2P)	0.0028574	40 7 0, 0 0 0	.17*-11.1997.
R1(4S3P,3P2S)	-0.0025459	37 8 -8,-12 0 0	.17*-11.213649384393.
R2(4S3P,3D2P)	-0.0042113	49 7 -5,-10 0 0	.17*-11.122211241.
R1(4S3D,3P2P)	-0.0102749	39 13 -9,-12 0 0	.17*-11.59.1048203803.
R2(4S3D,3D2S)	-0.0059100	51 8 -6,-10 2 0	.17*-11.103.97711.
R1(4P3S,3S2P)	0.0018687	25 8 -5,-12 2 0	.17*-11.81610988699.
R0(4P3S,3P2S)	0.0033386	38 7 1, 0 0 0	.17*-11.2087.
R1(4P3S,3D2P)	-0.0008291	36 8 -8,-12 0 0	.17*-11.98399536783.
R1(4P3P,3S2S)	-0.0003643	30 15 -5,-12 0 0	.17*-11.661591831.
R0(4P3P,3P2P)	0.0035945	51 6 1, 0 0 0	.17*-11.43.
R2(4P3P,3P2P)	0.0004487	43 6 -5,-10 2 0	.17*-11.61.268913.
R1(4P3P,3D2S)	-0.0045209	41 11 -8,-12 0 0	.17*-11.23.793637569.
R1(4P3D,3S2P)	-0.0055742	32 8 -6,-12 0 0	.17*-11.41.12908386471.
R2(4P3D,3P2S)	-0.0086949	43 7 -6,-10 0 0	.17*-11.97.587.79273.
R1(4P3D,3D2P)	-0.0084081	43 8 -9,-12 0 0	.17*-11.31.6362086993.
R3(4P3D,3D2P)	-0.0057269	51 6 -3, -6 0 0	.17*-11.587459.
R1(4D3S,3P2P)	-0.0049747	34 11 -7,-12 0 0	.17*-11.10162786783.
R0(4D3S,3D2S)	0.0039305	42 8 0, 0 0 2	.17*-11.61.
R2(4D3P,3S2P)	-0.0003927	38 11 -5,-10 0 0	.17*-11.57301369.
R1(4D3P,3P2S)	0.0010085	39 10 -7,-12 0 0	.17*-11.6308073217.
R0(4D3P,3D2P)	0.0034966	53 13 0, 0 0 0	.17*-11.
R2(4D3P,3D2P)	0.0006502	49 11 -6,-10 0 0	.17*-11.41.43.2659.
R2(4D3D,3S2S)	0.0053392	38 8 -6,-10 2 0	.17*-11.822931829.
R1(4D3D,3P2P)	0.0036020	41 11 -8,-12 0 0	.17*-11.14543503217.
R3(4D3D,3P2P)	-0.0001402	53 9 -2, -6 0 0	.17*-11.619.
R2(4D3D,3D2S)	-0.0121039	49 8 -7,-10 0 0	.17*-11.439.2309753.
R1(4F3S,3D2P)	0.0007875	40 11 -8,-13 0 0	.17*-11.571.20834327.

INTEGRAL	VALUE	2× (POWER OF FIRST SIX PRIMES)	ADDITIONAL FACTORS
R2(4F3P,3P2P)	0.0066946	45 13 -5,-11 0 0	.17*-11.76149079.
R1(4F3P,3D2S)	0.0105835	45 10 -8,-13 0 0	.17*-11.31*2.79.644843.
R3(4F3D,3S2P)	0.0069356	40 11 -2, -7 0 2	.17*-11.187987.
R2(4F3D,3P2S)	0.0159574	45 8 -6,-11 0 0	.17*-11.6326865263
R1(4F3D,3D2P)	0.0226018	47 11 -9,-13 0 0	.17*-11.199.339123383.
R3(4F3D,3D2P)	0.0110104	51 11 -3, -7 0 0	.17*-11.191693.
R0(4S3S,3S3S)	0.0090697	34-19-20,-14 0 2	.47.31051459.
R0(4S3P,3S3P)	0.0102670	48-19-20,-14 0 0	.31.571.9479.
R1(4S3P,3P3S)	0.0083824	46-17-20,-12 0 0	.31.420859.
R2(4S3P,3D3P)	0.0075392	45-19-19,-10 0 0	.3180607.
R0(4S3D,3S3D)	0.0125145	54-19-22,-14 0 0	.127823623.
R1(4S3D,3P3P)	0.0076667	55-17-21,-12 0 0	.19.53.1171.
R2(4S3D,3D3S)	0.0070878	58-19-20,-10 0 0	.31.2383.
R2(4S3D,3D3D)	0.0095602	45-19-21, -8 0 0	.89.32369.
R0(4P3S,3P3S)	0.0090125	41-16-21,-14 0 0	.29.47.73.7207.
R1(4P3P,3S3S)	0.0007039	39-14-21,-12 2 0	.97.4999.
R0(4P3P,3P3P)	0.0104995	59-18-21,-14 0 0	.19.241.1069.
R2(4P3P,3P3P)	0.0053935	37-18-19,-10 0 0	.21018857.
R1(4P3P,3D3S)	0.0074242	56-12-22,-12 0 0	.115823.
R1(4P3D,3S3P)	0.0011432	48-12-22,-12 0 0	.67.4259.
R2(4P3D,3P3S)	0.0024016	54-12-20,-10 0 0	.2141.
R0(4P3D,3P3D)	0.0129726	63-16-23,-14 0 0	.83.97.313.
R2(4P3D,3P3D)	0.0087803	37-16-21, -8 0 0	.313.26029.
R1(4P3D,3D3P)	0.0086515	59-14-23,-12 2 0	.29101.
R3(4P3D,3D3P)	0.0071624	49-16-23, -6 4 0	.613.
R0(4D3S,3D3S)	0.0078976	45-17-22,-14 0 2	.97.173.2789.
R2(4D3P,3S3P)	-0.0111228	32-17-19,-10 6 0	.106363.
R1(4D3P,3P3S)	-0.0108213	50-15-21,-12 0 0	.79.39727.
R0(4D3P,3D3P)	0.0093194	61-17-22,-14 0 0	.2804531.
R2(4D3P,3D3P)	0.0018505	43-17-20,-10 0 2	.89521.
R2(4D3D,3S3S)	-0.0073529	45-17-20,-10 0 0	.641.3607.
R2(4D3D,3S3D)	-0.0085313	32-17-21, -8 0 0	.29.2674531.
R1(4D3D,3P3P)	-0.0072081	57-15-22,-12 0 0	.263.1571.
R3(4D3D,3P3P)	-0.0028526	51-17-22, -6 0 0	.17.673.
R2(4D3D,3D3S)	-0.0014062	62-17-21,-10 0 0	.2731.
R0(4D3D,3D3D)	0.0131507	73-17-24,-14 0 2	.17.1399.
R2(4D3D,3D3D)	0.0090589	43-17-22, -8 0 0	.31.149.881.
R4(4D3D,3D3D)	0.0064590	57-13-24, -4 0 0	.257.
R2(4F3P,3P3P)	-0.0284167	39-17-19,-11 0 0	.47.1799599.
R1(4F3P,3D3S)	-0.0328722	52-15-22,-13 0 0	.28201049.
R3(4F3D,3S3P)	-0.0201473	38-17-22, -7 2 0	.1759133.
R2(4F3D,3P3S)	-0.0227341	52-17-20,-11 0 0	.31.53927.
R2(4F3D,3P3D)	-0.0271448	39-17-21, -9 0 0	.19.3037421.
R4(4F3D,3P3D)	-0.0171226	51-13-23, -5 0 0	.6449.
R1(4F3D,3D3P)	-0.0291752	67-15-23,-13 0 2	.17.1399.
R3(4F3D,3D3P)	-0.0188885	49-17-23, -7 0 0	.97.9241.
R0(4S3S,4S1S)	0.0004717	-8 7 0, 0-22 0	.46043177.
R0(4P3S,4P1S)	0.0004236	-8 11 0, 2-22 2	.19.2657.
R1(4P3P,4S1S)	-0.0021756	-3 12 5, 0-22 0	.67.643.
R2(4P3D,4P1S)	0.0009252	3 7 1, 0-22 0	.881.1013.
R0(4D3S,4D1S)	0.0000443	-8 17 0, 0-22 0	.23.773.
R1(4D3P,4P1S)	-0.0003574	-1 16 0, 0-22 0	.21977.
R2(4D3D,4S1S)	-0.0002139	5 13 2, 0-22 0	.1709.
R2(4D3D,4D1S)	0.0010585	3 7 -1, 0-22 0	.151.33811.
R0(4F3S,4F1S)	-0.0000004	-8 19 0, 0-22 0	.47.
R1(4F3P,4S1S)	0.0000006	-5 15 1, -1-22 0	.17.19.
R1(4F3P,4D1S)	0.0000053	-3 19 0, 1-22 0	.47.
R2(4F3D,4P1S)	-0.0001352	5 14 1, 1-22 0	.17.31.
R2(4F3D,4F1S)	0.0006140	3 7 1, -2-22 0	.4145717.
R0(4S3S,4S2S)	0.0018222	-59 7-10, 2 0 0	.13207247.
R0(4S3P,4S2P)	0.0018214	-60 8-10, 0 0 0	.67.479.2351.
R1(4P3S,4S2P)	-0.0004049	-59 13 -7, 2 0 0	.9721.
R0(4P3S,4P2S)	0.0021276	-59 11-10, 0 0 0	.359.33409.
R1(4P3P,4S2S)	-0.0059208	-60 12 -7, 0 2 0	.71.3121.
R0(4P3P,4P2P)	0.0022784	-60 12-10, 0 0 0	.10486877.
R2(4P3P,4P2P)	-0.0016312	-60 8 -2, 0 2 0	.9829.

INTEGRAL	VALUE	2× (POWER OF FIRST SIX PRIMES)						ADDITIONAL FACTORS
R1(4P3D,4S2P)	-0.0127343	-60	13	-8,	0	0	0	.6768127.
R2(4P3D,4P2S)	-0.0094813	-60	7	-3,	0	0	0	.641.3797.
R1(4D3S,4P2P)	-0.0020401	-59	19	-8,	0	0	0	.73.389.
R0(4D3S,4D2S)	0.0024547	-59	17	-10,	0	0	0	.512503.
R2(4D3P,4S2P)	-0.0030640	-60	14	-3,	0	4	0	.139.
R1(4D3P,4P2S)	-0.0064492	-60	16	-8,	0	0	0	.659653.
R0(4D3P,4D2P)	0.0022308	-60	20	-10,	0	0	0	.109.1163.
R2(4D3P,4D2P)	-0.0020529	-60	8	-6,	0	0	2	.261673.
R2(4D3D,4S2S)	-0.0033856	-60	13	-4,	0	0	0	.167.431.
R1(4D3D,4P2P)	-0.0098254	-60	23	-9,	0	0	0	.29.1657.
R3(4D3D,4P2P)	-0.0030878	-60	9	-1,	2	0	0	.7549.
R2(4D3D,4D2S)	-0.0126361	-60	7	-7,	0	0	0	.81093167.
R1(4F3S,4D2P)	-0.0024155	-59	20	-8,	1	2	0	.23.29.
R0(4F3S,4F2S)	0.0008083	-59	19	-10,	0	0	2	.4327.
R1(4F3P,4S2S)	0.0000893	-60	15	-5,	-1	0	0	.19.197.
R2(4F3P,4P2P)	0.0004581	-60	17	-4,	1	0	0	.409.
R1(4F3P,4D2S)	-0.0041089	-60	19	-8,	1	0	0	.19.1609.
R0(4F3P,4F2P)	0.0005810	-60	20	-10,	0	0	0	.137.241.
R2(4F3P,4F2P)	-0.0056639	-60	8	-4,	-2	0	0	.17.757.1021.
R3(4F3D,4S2P)	0.0021351	-60	14	-2,	3	0	0	.283.
R2(4F3D,4P2S)	0.0024910	-60	14	-5,	1	0	0	.25841.
R1(4F3D,4D2P)	-0.0034374	-60	20	-9,	1	0	0	.137.241.
R3(4F3D,4D2P)	0.0012213	-60	10	-1,	1	0	0	.4561.
R2(4F3D,4F2S)	-0.0143830	-60	7	-5,	-2	0	0	.129225667.
R0(4S3S,4S3S)	0.0449056	0	0	0,	-24	0	0	.83.223.33581.
R0(4S3P,4S3P)	0.0456956	0	0	0,	-24	0	0	.632486233.
R0(4S3D,4S3D)	0.0471664	0	0	0,	-24	0	0	.587.1112171.
R0(4P3S,4P3S)	0.0465115	0	0	0,	-24	0	0	.179.3596531.
R1(4P3P,4S3S)	0.0233907	13	7	1,	-24	0	0	.79.433.
R0(4P3P,4P3P)	0.0474929	0	0	0,	-24	2	0	.59760299.
R2(4P3P,4P3P)	0.0164507	6	2	2,	-24	0	2	.227.643.
R1(4P3D,4S3P)	0.0190807	20	7	2,	-24	0	0	.1103.
R2(4P3D,4P3S)	0.0118499	17	2	3,	-24	0	2	.1039.
R0(4P3D,4P3D)	0.0491249	0	0	2,	-24	0	0	.347.391903.
R2(4P3D,4P3D)	0.0148646	6	2	0,	-24	0	0	.8572693.
R0(4D3S,4D3S)	0.0498701	0	0	0,	-24	0	0	.690266569.
R2(4D3P,4S3P)	0.0107899	8	8	3,	-24	2	0	.937.
R1(4D3P,4P3S)	0.0213436	13	13	2,	-24	2	0	.47.
R0(4D3P,4D3P)	0.0508687	0	0	0,	-24	0	0	.704088409.
R2(4D3P,4D3P)	0.0185933	6	2	0,	-24	0	0	.10723109.
R2(4D3D,4S3S)	0.0093592	15	10	2,	-24	0	0	.19.31.
R2(4D3D,4S3D)	0.0084424	8	10	1,	-24	0	0	.13441.
R1(4D3D,4P3P)	0.0181726	20	15	1,	-24	0	0	.29.
R3(4D3D,4P3P)	0.0085238	10	3	1,	-22	2	2	.317.
R2(4D3D,4D3S)	0.0129914	17	2	1,	-24	2	0	.53.127.
R0(4D3D,4D3D)	0.0532957	0	0	0,	-24	0	0	.37.19937317.
R2(4D3D,4D3D)	0.0180026	6	2	-2,	-24	0	0	.51912229.
R4(4D3D,4D3D)	0.0094517	16	12	0,	-24	0	0	.701.
R0(4F3S,4F3S)	0.0559556	0	0	0,	-26	0	0	.29.186947627.
R1(4F3P,4S3S)	0.0047178	13	12	1,	-25	0	0	.1171.
R2(4F3P,4P3P)	0.0036309	8	11	2,	-25	2	0	.359.
R1(4F3P,4D3S)	0.0172699	13	18	2,	-25	0	0	.71.
R0(4F3P,4F3P)	0.0571095	0	0	0,	-26	0	2	.425636971.
R2(4F3P,4F3P)	0.0279256	6	2	4,	-26	0	0	.83.54331.
R3(4F3D,4S3P)	-0.0016969	10	8	4,	-23	0	0	.137.
R2(4F3D,4P3S)	0.0030006	15	13	3,	-25	0	0	.43.
R2(4F3D,4P3D)	-0.0005096	8	11	0,	-25	0	0	.17.163.
R4(4F3D,4P3D)	-0.0022670	14	11	0,	-25	0	0	.23.67.
R1(4F3D,4D3P)	0.0135377	20	18	1,	-25	2	0	
R3(4F3D,4D3P)	0.0063207	10	4	1,	-23	0	0	.51347.
R2(4F3D,4F3S)	0.0220450	17	2	5,	-26	0	0	.127.277.
R0(4F3D,4F3D)	0.0593978	0	0	2,	-26	0	0	.115099798?.
R2(4F3D,4F3D)	0.0252483	6	2	2,	-26	0	0	.20395697.
R4(4F3D,4F3D)	0.0149772	16	10	0,	-26	0	0	.23327.
R0(4S4S,1S1S)	0.0023396	12	2	-20,	2	0	0	.17.
R1(4P4P,1S1S)	0.0055325	12	4	-22,	2	0	0	.67.

INTEGRAL	VALUE	2× (POWER OF FIRST SIX PRIMES)	ADDITIONAL FACTORS
R2(4D4D,1S1S)	0.0006593	12 0-22, 0 0 0	.503.
R3(4F4F,1S1S)	0.0000144	12 0-22, 0 2 0	
R0(4S4S,2S1S)	0.0008416	-31 2 0, 0 0 2	
R1(4S4P,2P1S)	-0.0023241	-31 -8 -9, 0 0 2	.937819.
R0(4P4S,2P1S)	0.0007238	-31 2 3, 0 0 0	
R1(4P4P,2S1S)	-0.0005122	-31 -6 -8, 0 0 0	.71.5641.
R2(4P4D,2P1S)	0.0011462	-31 -6 -6, 0 0 0	.179261.
R1(4D4P,2P1S)	0.0041724	-31 -8 -8, 0 2 0	.889871.
R2(4D4D,2S1S)	-0.0016831	-31 -6 -6, 0 0 0	.263239.
R3(4D4F,2P1S)	0.0002991	-31 -7 2, 5 0 0	
R2(4F4D,2P1S)	0.0006100	-31 -7 -6, -1 0 0	.409.1069.
R3(4F4F,2S1S)	-0.0001284	-31 -6 -2, 0 2 0	.73.
R0(4S4S,2S2S)	0.0023935	6-22 0, 0 0 0	.53.
R1(4S4S,2P2P)	0.0032415	8-26 0, 0 0 0	.17.19.
R1(4P4S,2S2P)	0.0017840	6-24 1, 0 0 0	.53.
R0(4P4S,2P2S)	0.0025245	6-22 5, 0 0 0	
R1(4P4P,2S2S)	0.0029354	6-22 2, 0 0 2	
R0(4P4P,2P2P)	0.0031612	8-22 2, 2 0 0	
R2(4P4P,2P2P)	0.0040042	8-24 0, 2 0 0	.19.
R1(4D4S,2P2P)	-0.0036802	12-26 1, 0 0 0	.41.
R2(4D4P,2S2P)	0.0001656	6-24 0, 0 2 0	
R1(4D4P,2P2S)	0.0018817	6-24 6, 0 0 0	
R2(4D4D,2S2S)	0.0105524	6-24 0, 0 0 0	.701.
R1(4D4D,2P2P)	0.0119926	8-26 2, 0 0 0	.239.
R3(4D4D,2P2P)	0.0073762	8-24 2, 4 0 0	
R2(4F4P,2P2P)	-0.0010643	10-17 0, -1 0 0	
R3(4F4D,2S2P)	-0.0040240	6-25 4, 3 0 0	
R2(4F4D,2P2S)	-0.0048584	6-23 0, -1 0 0	.17.29.
R3(4F4F,2S2S)	0.0039892	6-24 2, 0 0 0	.53.
R2(4F4F,2P2P)	0.0030006	8-26 0, 0 0 2	.23.
R4(4F4F,2P2P)	0.0019569	8-24 2, 0 0 2	
R0(4S4S,3S1S)	0.0004520	12 7 2, 2-22 0	.1231.
R1(4S4P,3P1S)	-0.0015216	17 12 -9,-12-22 0	.270452997587.
R2(4S4D,3D1S)	-0.0001683	21 7 -6,-10-22 0	.23.29.2233867.
R0(4P4S,3P1S)	0.0003932	17 8 1, 0-22 0	.29.59.
R1(4P4P,3S1S)	-0.0105836	12 13 -6,-12-22 0	.549519985129.
R1(4P4P,3D1S)	0.0000032	19 13 -9,-12-22 0	.29.5617163.
R2(4P4D,3P1S)	0.0000901	17 8 -6,-10-22 0	.18414644557.
R3(4P4F,3D1S)	-0.0000392	21 10 -3, -7-22 0	.322397.
R0(4D4S,3D1S)	0.0000278	21 11 0, 0-22 2	
R1(4D4P,3P1S)	0.0001007	17 16 -8,-12-22 0	.9721878977.
R2(4D4D,3S1S)	-0.0005550	12 11 -6,-10-22 0	.12350696263.
R2(4D4D,3D1S)	0.0009676	19 11 -7,-10-22 2	.41.227.35171.
R3(4D4F,3P1S)	0.0000308	17 13 -2, -7-22 0	.71.1229.
R1(4F4P,3D1S)	0.0018544	21 18 -9,-13-22 0	.73.110608441.
R2(4F4D,3P1S)	-0.0003685	17 11 -6,-11-22 0	.3835360777.
R3(4F4F,3S1S)	0.0000418	12 15 -2, -8-22 0	.590099.
R3(4F4F,3D1S)	0.0001291	19 17 -3, -8-22 0	.120121.
R0(4S4S,3S2S)	0.0013277	-55 7 0, 0 0 0	.17.317.
R1(4S4S,3P2P)	0.0006698	-56 -4 0,-12 0 0	.233.817111357.
R0(4S4P,3S2P)	0.0013139	-55 11 3, 0 0 0	.53.
R1(4S4P,3P2S)	-0.0019586	-56 -2 1,-12 0 0	.82985643287.
R2(4S4P,3D2P)	-0.0025100	-56 1 0,-10 0 0	.6537975023.
R1(4S4D,3P2P)	-0.0054149	-56 -4 1,-12 0 0	.688300805903.
R2(4S4D,3D2S)	-0.0019392	-56 1 0,-10 0 0	.5015260823.
R2(4S4F,3D2P)	0.0002275	-56 0 0, -9 0 0	.3879219671.
R1(4P4S,3S2P)	0.0007824	-55 -3 3,-12 0 0	.8119848229.
R0(4P4S,3P2S)	0.0015553	-56 8 3, 0 0 0	.461.
R1(4P4S,3D2P)	-0.0009800	-56 -3 0,-12 0 0	.83.89.21770101.
R1(4P4P,3S2S)	-0.0007851	-55 -1 4,-12 0 0	.1214692327.
R0(4P4P,3P2P)	0.0016973	-56 12 8, 0 0 0	
R2(4P4P,3P2P)	-0.0001297	-56 2 0,-10 0 0	.195069559.
R1(4P4P,3D2S)	-0.0031028	-56 -1 1,-12 2 0	.6900467881.
R1(4P4D,3S2P)	-0.0628979	-55 -3 4,-12 0 0	.15408002191.
R2(4P4D,3P2S)	-0.0044655	-56 2 0,-10 0 0	.6715513279.
R1(4P4D,3D2P)	-0.0040145	-56 -3 1,-12 0 0	.53.79.70364257.

INTEGRAL	VALUE	2× (POWER OF FIRST SIX PRIMES)						ADDITIONAL FACTORS
R3(4P4D,3D2P)	-0.0024709	-56	3	3,	4	0	0	.233.
R2(4P4F,3P2P)	0.0024678	-56	1	0,	-9	0	0	.2429608543.
R3(4P4F,3D2S)	0.0033657	-56	4	1,	-7	0	0	.113.360541.
R1(4D4S,3P2P)	-0.0006378	-56	0	1,	-12	0	0	.9007572311.
R0(4D4S,3D2S)	0.0017326	-56	11	2,	0	0	2	.17.
R2(4D4P,3S2P)	-0.0005228	-55	5	0,	-10	0	0	.61.433.4051.
R1(4D4P,3P2S)	-0.0000005	-56	2	2,	-12	0	0	.317.3359.
R0(4D4P,3D2P)	0.0014199	-56	19	3,	0	0	0	
R2(4D4P,3D2P)	-0.0006542	-56	5	-1,	-10	0	0	.17.24904727.
R2(4D4D,3S2S)	0.0019705	-55	5	0,	-10	0	0	.47.8580031.
R1(4D4D,3P2P)	0.0014251	-56	0	2,	-12	0	0	.103.87390131.
R3(4D4D,3P2P)	-0.0003204	-56	6	2,	4	0	2	
R2(4D4D,3D2S)	-0.0071769	-56	5	-1,	-10	0	0	.4644626479.
R2(4D4F,3S2P)	-0.0018467	-55	4	0,	-9	0	0	.41.67.90067.
R3(4D4F,3P2S)	-0.0001307	-56	7	2,	-7	2	0	.12377.
R2(4D4F,3D2P)	0.0029021	-56	4	-1,	-9	0	2	.94580011.
R4(4D4F,3D2P)	0.0021254	-56	14	7,	-5	4	0	
R1(4F4S,3D2P)	0.0008466	-56	0	0,	-13	0	0	.70740012977.
R2(4F4P,3P2P)	0.0034317	-56	5	0,	-11	0	2	.202135573.
R1(4F4P,3D2S)	0.0060931	-56	2	1,	-13	0	0	.607.125032123.
R3(4F4D,3S2P)	0.0016202	-55	8	2,	3	0	0	.41.
R2(4F4D,3P2S)	0.0050726	-56	5	0,	-11	2	0	.43.8211953.
R1(4F4D,3D2P)	0.0102931	-56	0	1,	-13	2	0	.41.137.6225047.
R3(4F4D,3D2P)	0.0043112	-56	10	3,	3	0	0	.23.
R3(4F4F,3S2S)	-0.0057705	-55	9	2,	-8	0	0	.563.6659.
R2(4F4F,3P2P)	-0.0060928	-56	4	0,	-10	0	2	.709.331369.
R4(4F4F,3P2P)	-0.0036773	-56	16	2,	-6	0	0	.10321.
R3(4F4F,3D2S)	-0.0068310	-56	11	1,	-8	0	0	.4678067.
R0(4S4S,3S3S)	0.0037748	12	6	0,	-28	0	0	.1481573.
R1(4S4S,3P3P)	0.0049745	24	8	0,	-28	0	0	.10169.
R2(4S4S,3D3D)	0.0041737	28	14	0,	-28	0	0	.79.
R1(4P4S,3S3P)	0.0038910	17	11	3,	-28	0	0	.1549.
R0(4P4S,3P3S)	0.0040043	17	7	3,	-28	0	0	.14347.
R2(4P4S,3P3D)	0.0033166	24	7	0,	-28	0	0	.11743.
R1(4P4S,3D3P)	0.0041407	24	15	0,	-28	0	0	.181.
R1(4P4P,3S3S)	0.0042690	12	8	2,	-28	0	0	.37.3019.
R0(4P4P,3P3P)	0.0044279	24	6	2,	-28	0	0	.5431.
R2(4P4P,3P3P)	0.0053039	24	6	0,	-28	2	0	.2957.
R1(4P4P,3D3S)	0.0030852	19	8	3,	-28	0	0	.3191.
R1(4P4P,3D3D)	0.0046238	28	8	0,	-28	0	0	.17.139.
R3(4P4P,3D3D)	0.0047973	28	6	2,	-28	0	0	.1471.
R2(4D4S,3S3D)	0.0008383	21	8	0,	-28	0	0	.37.131.
R1(4D4S,3P3P)	0.0009123	26	10	1,	-28	0	0	.139.
R0(4D4S,3D3S)	0.0038906	21	8	2,	-28	2	0	.409.
R2(4D4S,3D3D)	0.0021820	26	8	-1,	-28	0	0	.4987.
R2(4D4P,3S3P)	0.0024496	17	11	0,	-28	0	0	.10903.
R1(4D4P,3P3S)	0.0032499	17	11	2,	-28	2	0	.263.
R1(4D4P,3P3D)	0.0014380	24	11	1,	-28	2	0	.23.
R3(4D4P,3P3D)	0.0028173	24	9	1,	-28	0	0	.1487.
R0(4D4P,3D3P)	0.0043822	24	13	1,	-28	0	0	.257.
R2(4D4P,3D3P)	0.0048642	24	11	-1,	-28	2	0	.389.
R2(4D4D,3S3S)	0.0081813	12	14	0,	-28	0	0	.29.1367.
R1(4D4D,3P3P)	0.0062738	24	14	4,	-28	0	0	.19.
R3(4D4D,3P3P)	0.0056574	24	12	2,	-28	0	0	.257.
R2(4D4D,3D3S)	0.0028809	19	14	-1,	-28	0	0	.31.99.
R0(4D4D,3D3D)	0.0052304	28	18	0,	-28	2	0	
R2(4D4D,3D3D)	0.0071957	28	16	-2,	-28	0	0	.227.
R4(4D4D,3D3D)	0.0058643	28	16	0,	-28	0	0	.37.
R2(4F4S,3P3D)	-0.0055966	24	8	0,	-29	0	0	.30269.
R1(4F4S,3D3P)	-0.0065902	24	10	0,	-29	0	0	.109*2.
R3(4F4P,3S3D)	-0.0026075	21	11	1,	-29	0	0	.3433.
R2(4F4P,3P3P)	-0.0014642	28	13	0,	-29	0	0	.127.
R1(4F4P,3D3S)	-0.0005659	21	11	3,	-29	0	0	.149.
R1(4F4P,3D3D)	-0.0066502	26	11	0,	-29	0	0	.3461.
R3(4F4P,3D3D)	-0.0046596	26	11	4,	-29	0	0	.97.
R3(4F4D,3S3P)	-0.0071990	17	14	2,	-29	0	2	.251.

INTEGRAL	VALUE	2× (POWER OF FIRST SIX PRIMES)					ADDITIONAL FACTORS
R2(4F4D,3P3S)	0.0106416	17	16	0,-29	0	0	.8039.
R2(4F4D,3P3D)	0.0014087	24	14	-1,-29	0	0	.631.
R4(4F4D,3P3D)	0.0019088	24	18	1,-29	0	0	.19.
R1(4F4D,3D3P)	0.0077805	24	14	1,-29	0	0	.17.41.
R3(4F4D,3D3P)	0.0040298	24	14	1,-29	0	0	.19*2.
R3(4F4F,3S3S)	0.0212939	12	16	2,-30	0	0	.179.269.
R2(4F4F,3P3P)	0.0248857	24	14	0,-30	4	0	.109.
R4(4F4F,3P3P)	0.0170666	24	20	2,-30	0	0	.67.
R3(4F4F,3D3S)	0.0172894	19	16	1,-30	0	0	.7727.
R1(4F4F,3D3D)	0.0262122	28	14	0,-30	0	0	.23.151.
R3(4F4F,3D3D)	0.0159628	28	18	2,-30	0	0	.47.
R5(4F4F,3D3D)	0.0112079	28	20	2,-30	2	0	
R0(4S4S,4S1S)	0.0002920	22		2-10,-22	0	0	.293677.
R0(4P4S,4P1S)	0.0002547	22		2-10,-22	0	0	.19.97.139.
R1(4P4P,4S1S)	-0.0013034	20		4 -8,-22	0	0	.19.9199.
R2(4P4D,4P1S)	0.0006526	20		0 -3,-22	0	0	.73.193.
R0(4D4S,4D1S)	0.0000217	24		2-10,-22	2	0	.991.
R1(4D4P,4P1S)	-0.0001757	20		4 -9,-22	0	0	.19.47.59.
R2(4D4D,4S1S)	-0.0001672	26		0 -4,-22	0	0	.1009.
R2(4D4D,4D1S)	0.0007293	20		0 -7,-22	0	0	.167.2357.
R3(4D4F,4P1S)	-0.0000113	30	-1	-1,-21	0	0	
R0(4F4S,4F1S)	-0.0000005	26		6-10,-24	0	0	.101.
R1(4F4P,4S1S)	-0.0000042	18		3 -6,-23	0	0	.1031.
R1(4F4P,4D1S)	0.0000079	24		9 -9,-23	0	0	.101.
R2(4F4D,4P1S)	-0.0000869	24	-1	-5,-23	0	2	.827.
R2(4F4D,4F1S)	0.0004039	18		0 -5,-24	0	2	.29.1619.
R3(4F4F,4S1S)	0.0000157	26		0 -2,-22	0	0	.19.
R3(4F4F,4D1S)	0.0000383	18		0 -1,-22	0	0	.331.
R0(4S4S,4S2S)	0.0008444	19	-12	-22, 0	0	2	.31.103.
R0(4S4P,4S2P)	0.0008349	21	-12	-23, 0	0	0	.45887.
R1(4P4S,4S2P)	-0.0001774	19	-8	-23, 0	2	0	.197.
R0(4P4S,4P2S)	0.0009867	19	-12	-24, 0	0	0	.409.593.
R1(4P4P,4S2S)	-0.0029707	17	-6	-24, 2	0	0	.7727.
R0(4P4P,4P2P)	0.0010710	25	-12	-25, 0	2	0	.6689.
R2(4P4P,4P2P)	-0.0006992	17	-6	-23, 0	0	0	.5693.
R1(4P4D,4S2P)	-0.0055447	25	-8	-24, 0	0	0	.23.823.
R2(4P4D,4P2S)	-0.0034661	17	-6	-23, 0	0	4	.167.
R2(4P4F,4P2P)	0.0033655	19	-7	-23, -1	0	0	.62791.
R1(4D4S,4P2P)	-0.0011463	19	-8	-24, 0	0	0	.31307.
R0(4D4S,4D2S)	0.0010846	21	-12	-24, 0	0	0	.17.7841.
R2(4D4P,4S2P)	-0.0013994	23	-6	-22, 4	0	2	
R1(4D4P,4P2S)	-0.0031764	17	-6	-25, 0	0	0	.17.7607.
R0(4D4P,4D2P)	0.0009224	25	-12	-25, 0	0	0	.127.499.
R2(4D4P,4D2P)	-0.0011226	17	-4	-23, 0	2	0	.277.
R2(4D4D,4S2S)	-0.0003449	23	-6	-22, 0	0	0	.157.
R1(4D4D,4P2P)	-0.0037895	21	-8	-25, 0	0	0	.251.461.
R3(4D4D,4P2P)	-0.0008280	25	-6	-25, 4	0	0	.43.
R2(4D4D,4D2S)	-0.0051459	17	-4	-23, 0	0	0	.13967.
R2(4D4F,4S2P)	0.0016602	23	-7	-22, -1	0	0	.3463.
R3(4D4F,4P2S)	0.0024294	25	-5	-25, 1	0	0	.19.71.
R2(4D4F,4D2P)	0.0041950	19	-5	-23, 1	0	0	.3727.
R4(4D4F,4D2P)	0.0021820	19		1-25, 1	0	0	.359.
R1(4F4S,4D2P)	-0.0009774	23	-9	-24, 1	0	0	.17.257.
R0(4F4S,4F2S)	0.0001415	23	-12	-24, 0	0	0	.8693.
R1(4F4P,4S2S)	0.0005549	15	-7	-24, -1	0	0	.29.31.103.
R2(4F4P,4P2P)	0.0007459	23	-7	-23, 3	0	0	.71.
R1(4F4P,4D2S)	-0.0013091	21	-7	-25, 1	2	2	.61.
R0(4F4P,4F2P)	0.0000629	29	-12	-25, 0	0	0	.23.47.
R2(4F4P,4F2P)	-0.0027206	15	-4	-23, -2	0	0	.19.5441.
R3(4F4D,4S2P)	0.0009819	23	-7	-24, 3	2	0	.19.
R2(4F4D,4P2S)	0.0017702	21	-7	-23, 3	0	0	.337.
R1(4F4D,4D2P)	-0.0004326	27	-9	-25, 1	0	0	.23.47.
R3(4F4D,4D2P)	0.0015002	25	-5	-25, 5	0	0	.17.
R2(4F4D,4F2S)	-0.0044006	15	-4	-23, -2	0	2	.19.677.
R3(4F4F,4S2S)	-0.0012026	23	-6	-24, 2	0	0	.17.23.
R2(4F4F,4P2P)	-0.0004840	25	-8	-23, 0	0	0	.739.

INTEGRAL	VALUE	2× (POWER OF FIRST SIX PRIMES)	ADDITIONAL FACTORS
R4(4F4F,4P2P)	-0.0007865	19 0-25, 0 0 0	.593.
R3(4F4F,4D2S)	0.0005483	15 -4-25, 0 0 0	.23.647.
R2(4F4F,4F2P)	0.0055587	17 -5-23, 3 0 0	.17.83.
R4(4F4F,4F2P)	0.0031279	19 -1-25, -1 0 0	.101.107.
R0(4S4S,4S3S)	0.0028723	22 7 6,-14 0-26	.59842448873.
R0(4S4P,4S3P)	0.0029020	29 8 1,-14 0-26	.17.719.14111161.
R0(4S4D,4S3D)	0.0026514	33 11 2,-14 0-26	.101.33571189.
R1(4P4S,4S3P)	0.0001131	27 12 1,-12 0-26	.213361807.
R0(4P4S,4P3S)	0.0032076	22 11 0,-14 0-26	.19.53.921725807.
R2(4P4S,4P3D)	0.0002687	31 7 1,-10 0-26	.17.16602917.
R1(4P4P,4S3S)	-0.0048036	20 13 2,-12 0-26	.17.1557439931.
R1(4P4P,4S3D)	0.0008528	33 13 1,-12 6-26	.87251.
R0(4P4P,4P3P)	0.0033135	33 12 3,-14 0-24	.17.4950707.
R2(4P4P,4P3P)	-0.0025311	25 8 1,-10 0-24	.23.31.277.4783.
R1(4P4D,4S3P)	-0.0099778	33 16 2,-12 0-26	.116337347.
R2(4P4D,4P3S)	-0.0103058	20 11 1,-10 0-26	.19.2865045811.
R0(4P4D,4P3D)	0.0030345	35 19 2,-14 0-26	.23954927.
R2(4P4D,4P3D)	-0.0025225	31 11 0,-10 0-26	.19.34649557.
R1(4P4F,4S3D)	-0.0185406	33 20 1,-13 0-26	.142833839.
R2(4P4F,4P3P)	-0.0155022	27 11 1,-11 0-26	.17.983.1145873.
R2(4D4S,4S3D)	-0.0004293	33 13 2,-10 0-26	.3734693.
R1(4D4S,4P3P)	-0.0008304	27 16 0,-12 0-26	.17.67.131.2609.
R0(4D4S,4D3S)	0.0038007	24 17 0,-14 2-26	.185154310l.
R2(4D4S,4D3D)	0.0001967	33 7 -1, -8 0-26	.29.271.9391.
R2(4D4P,4S3P)	-0.0040475	31 14 2,-10 0-26	.53.767153.
R1(4D4P,4P3S)	-0.0054655	20 19 1,-12 0-26	.2494854731.
R1(4D4P,4P3D)	0.0005424	31 23 2,-12 0-26	.271841.
R3(4D4P,4P3D)	-0.0010422	39 9 2, -6 0-26	.43.47.103.
R0(4D4P,4D3P)	0.0038093	33 20 1,-14 0-26	.77643617.
R2(4D4P,4D3P)	-0.0027887	25 8 -1, -8 0-26	.9664578653.
R2(4D4D,4S3S)	-0.0085172	26 21 6,-10 0-26	.23.41.439.
R2(4D4D,4S3D)	-0.0039951	39 19 1,-10 0-26	.19.29.653.
R1(4D4D,4P3P)	-0.0095765	29 24 3,-12 0-26	.43.59.977.
R3(4D4D,4P3P)	-0.0061807	33 12 1, -6 0-26	.179.23743.
R2(4D4D,4D3S)	-0.0118978	20 11 -1, -8 2-26	.4080837203.
R0(4D4D,4D3D)	0.0037648	43 23 2,-14 0-26	.179.1153.
R2(4D4D,4D3D)	-0.0021217	31 11 -2, -8 0-26	.395536051.
R4(4D4D,4D3D)	-0.0020662	33 21 2, -4 0-26	.647.
R2(4D4F,4S3P)	-0.0119729	31 19 2,-11 0-26	.53.385159.
R3(4D4F,4P3S)	-0.0114765	30 14 1, -7 0-26	.19684949.
R1(4D4F,4P3D)	-0.0172525	43 24 2,-13 0-26	.179.1153.
R3(4D4F,4P3D)	-0.0084005	35 16 4, -7 0-26	.75941.
R2(4D4F,4D3P)	-0.0175926	27 11 -1, -9 0-26	.29.199.2689651.
R4(4D4F,4D3P)	-0.0103140	27 23 1, -5 0-26	.50951.
R2(4F4S,4P3D)	-0.0031017	33 14 1, -9 0-26	.101.130363.
R1(4F4S,4D3P)	-0.0022779	31 19 0,-11 0-26	.19418423.
R0(4F4S,4F3S)	0.0049357	26 19 0,-14 0-26	.421.10470641.
R2(4F4S,4F3D)	0.0036502	31 7 1,-10 0-26	.3834436877.
R2(4F4P,4S3D)	-0.0040367	33 14 1, -5 0-26	.349709.
R2(4F4P,4P3P)	-0.0054966	31 17 1, -9 0-26	.157.57203.
R1(4F4P,4D3S)	-0.0061517	24 20 1,-11 0-26	.31.67.73757.
R1(4F4P,4D3D)	-0.0016773	37 20 2,-11 0-26	.179.1153.
R3(4F4P,4D3D)	-0.0033075	29 10 2, -7 0-26	.17.1899523.
R0(4F4P,4F3P)	0.0046578	37 20 3,-14 0-26	.23.179.1153.
R2(4F4P,4F3P)	-0.0010432	23 8 1,-10 0-26	.10122962189.
R3(4F4D,4S3P)	-0.0048436	31 17 2, -5 0-26	.72229.
R2(4F4D,4P3S)	-0.0073349	24 20 1, -9 0-26	.19.1373363.
R2(4F4D,4P3D)	-0.0052789	39 22 0, -9 0-26	.53.1459.
R4(4F4D,4P3D)	-0.0043270	33 25 2, -3 0-26	.887.
R1(4F4D,4D3P)	-0.0097444	35 23 3,-11 0-26	.179.1153.
R3(4F4D,4D3P)	-0.0079425	31 13 1, -7 0-26	.16685003.
R2(4F4D,4F3S)	-0.0124368	19 11 1,-10 0-26	.139907320009.
R1(4F4D,4F3D)	0.0037648	43 23 2,-14 0-26	.179.1153.
R2(4F4D,4F3D)	-0.0033497	29 11 0,-10 0-26	.1748449243.
R4(4F4D,4F3D)	-0.0034813	33 19 4, -6 0-26	.19.241.
R3(4F4F,4S3S)	-0.0029174	26 19 2, -6 0-26	.127.1709.

INTEGRAL	VALUE	2× (POWER OF FIRST SIX PRIMES)	ADDITIONAL FACTORS
R3(4F4F,4S3D)	-0.0002593	37 19 1, -6 0-26	.953.
R2(4F4F,4P3P)	-0.0059231	33 20 1,-10 0-26	.211.11677.
R4(4F4F,4P3P)	-0.0032335	27 22 1, -4 0-26	.10457.
R3(4F4F,4D3S)	-0.0117612	18 15 1, -8 0-26	.1972167817.
R1(4F4F,4D3D)	-0.0131768	41 23 2,-12 0-26	.179.1153.
R3(4F4F,4D3D)	-0.0069295	29 17 2, -8 0-26	.19.201451.
R5(4F4F,4D3D)	-0.0045247	37 21 0, -2 2-26	.23.
R2(4F4F,4F3P)	-0.0255578	25 11 1,-11 0-26	.43.59.61.163.2503.
R4(4F4F,4F3P)	-0.0170608	27 21 1, -7 0-26	.47.37657.
R0(4S4S,4S4S)	0.0372715	-38 0 0, 0 0 0	.19541.
R0(4P4S,4P4S)	0.0380383	-38 0 0, 4 2 0	.37.
R1(4P4P,4S4S)	0.0244617	-38 6 4, 0 0 0	.19.
R0(4P4P,4P4P)	0.0389347	-38 0 0, 0 0 0	.137.149.
R2(4P4P,4P4P)	0.0199223	-38 0 2, 0 0 0	.2089.
R0(4D4S,4D4S)	0.0394688	-38 0 0, 0 0 0	.20693.
R2(4D4P,4S4P)	0.0169106	-38 0 3, 0 0 2	.61.
R1(4D4P,4P4S)	0.0228389	-38 4 3, 2 0 0	.17.
R0(4D4P,4D4P)	0.0405102	-38 0 0, 0 0 0	.67.317.
R2(4D4P,4D4P)	0.0200634	-38 0 0, 0 0 0	.67.157.
R2(4D4D,4S4S)	0.0154209	-38 2 2, 4 2 0	
R1(4D4D,4P4P)	0.0219898	-38 6 0, 2 0 0	.61.
R3(4D4D,4P4P)	0.0147266	-38 0 0, 2 0 0	.1103.
R2(4D4D,4D4S)	0.0168167	-38 0 1, 0 0 0	.3943.
R0(4D4D,4D4D)	0.0426731	-38 0 0, 0 0 2	.1721.
R2(4D4D,4D4D)	0.0215733	-38 2 -2, 2 0 0	.2693.
R4(4D4D,4D4D)	0.0147800	-38 6 0, 2 0 0	.41.
R0(4F4S,4F4S)	0.0414715	-38 0 0, 0 0 0	.17.1279.
R1(4F4P,4S4S)	0.0116687	-38 3 2, 1 0 0	.89.
R2(4F4P,4P4P)	0.0117269	-38 -1 4, 3 0 0	.23.
R1(4F4P,4D4S)	0.0184696	-38 7 3, 3 0 0	
R0(4F4P,4F4P)	0.0426731	-38 0 0, 0 0 2	.1721.
R2(4F4P,4F4P)	0.0196825	-38 0 2, -2 0 0	.14447.
R3(4F4D,4S4P)	0.0089840	-38 -1 1, 3 0 0	.197.
R2(4F4D,4P4S)	0.0112381	-38 1 5, 1 0 0	.23.
R2(4F4D,4P4D)	0.0120125	-38 -1 0, 3 0 0	.19.31.
R4(4F4D,4P4D)	0.0092038	-38 9 0, 1 0 2	
R1(4F4D,4D4P)	0.0181716	-38 7 0, 3 2 0	
R3(4F4D,4D4P)	0.0123329	-38 1 0, 1 0 0	.17.83.
R2(4F4D,4F4S)	0.0160820	-38 0 3, -2 0 0	.5279.
R0(4F4D,4F4D)	0.0453167	-38 0 0, 0 0 0	.23.1033.
R2(4F4D,4F4D)	0.0218639	-38 2 0, 0 0 0	.3821.
R4(4F4D,4F4D)	0.0138531	-38 6 0, 0 0 0	.269.
R3(4F4F,4S4S)	0.0082111	-38 2 2, 2 0 0	.41.
R2(4F4F,4P4P)	0.0103855	-38 4 2, 0 4 0	
R4(4F4F,4P4P)	0.0086002	-38 6 0, 0 0 0	.167.
R3(4F4F,4D4S)	0.0096280	-38 0 1, 2 0 0	.17*2.
R1(4F4F,4D4D)	0.0171833	-38 4 0, 2 2 2	
R3(4F4F,4D4D)	0.0132009	-38 4 0, 0 0 0	.769.
R5(4F4F,4D4D)	0.0101337	-38 2 0, 2 2 0	.23.
R2(4F4F,4F4P)	0.0101620	-38 -1 2, -1 0 0	.19.257.
R4(4F4F,4F4P)	0.0069338	-38 5 0, -1 0 0	.617.
R0(4F4F,4F4F)	0.0502262	-38 0 0, 0 0 0	.17.1549.
R2(4F4F,4F4F)	0.0231402	-38 10 4, -2 0 0	.17.
R4(4F4F,4F4F)	0.0138018	-38 4 0, -2 2 0	.17.41.
R6(4F4F,4F4F)	0.0139103	-38 2 0, 0 2 2	.17.